Postgraduate Papers in Chemistry under NEP-2020

EFFECTIVE FROM JULY 2026

M.Sc. CHEMISTRY (M26) under NEP-2020

Specialization in: Inorganic or Organic or Physical or Materials

Department of Chemistry (Faculty of Sciences)
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Jamia Nagar, New Delhi-110025

Course Structure for M.Sc. Chemistry under NEP-2020 (Effective 2026–27)

- **Core Branches/Streams:** Inorganic, Organic, Physical, Materials.
- **Semesters I & II:** Common core theory + Elective + *separate practicals for each stream.*
- **Semesters III & IV:** Advanced core, branch/specialization papers and **Project/Dissertation**.
- **Paper Types:**
  - DSC: Discipline Specific Core (Core)
  - DSE: Discipline Specific Elective (Branch papers)
  - OE: Open/Generic Elective
  - RM: Research Methodology
  - RC: Research Component (Project/Dissertation, Seminar, Viva)

Semester-wise Distribution of Papers in M.Sc. Chemistry (NEP-2020)

Sem	Paper Code	Course Title	Paper Type	L–P / Credits
				Common Papers for all branches
I	MCH-101	Advanced Inorganic Chemistry–I	Theory (DSC)	3–0 / 3
	MCH-101L	Inorganic Chemistry Lab–I	Practical	0–4 / 2
	MCH-102	Stereochemistry and Reactive Intermediates	Theory (DSC)	3–0 / 3
	MCH-102L	Organic Chemistry Lab–I	Practical	0–4 / 2
	MCH-103	Mathematical Methods & Quantum Chemistry	Theory (DSC)	3–0 / 3
	MCH-103L	Physical Chemistry Lab–I	Practical	0–4 / 2
	MCH-104	Materials Chemistry–I	Theory (DSC)	3–0 / 3
	MCH-104L	Materials Chemistry Lab–I	Practical	0–4 / 2
	MCH-151	Molecular Spectroscopy	Elective (OE)	3–0 / 3
			Total L–P/Credits in Semester I	**15–16/23**
				Common Papers for all branches
II	MCH-201	Advanced Inorganic Chemistry–II	Theory (DSC)	3–0 / 3
	MCH-201L	Inorganic Chemistry Lab–II	Practical	0–4 / 2
	MCH-202	Pericyclic Reactions and Photochemistry	Theory (DSC)	3–0 / 3
	MCH-202L	Organic Chemistry Lab–II	Practical	0–4 / 2
	MCH-203	Irreversible & Statistical Thermodynamics	Theory (DSC)	3–0 / 3
	MCH-203L	Physical Chemistry Lab–II	Practical	0–4 / 2
	MCH-204	Materials Chemistry–II	Theory (DSC)	3–0 / 3
	MCH-204L	Materials Chemistry Lab–II	Practical (Lab)	0–4 / 2
	MCH-251	Interpretative spectroscopy	Elective (OE)	3–0 / 3
			Total L–P/Credits in Semester II	**15-16/23**
				Inorganic Branch Special (Spl.) Papers
III	MCH-3I1	Chemical Applications of Group Theory	Inorganic Spl. (DSE)	3–0 / 3
	MCH-3I2	Advanced Inorganic Reaction Mechanism	Inorganic Spl. (DSE)	3–0 / 3
	MCH-3I3	Advanced Organometallic Chemistry-I	Inorganic Spl. (DSE)	3–0 / 3
	MCH-3I4	Advanced Bio-inorganic Chemistry-I	Inorganic Spl. (DSE)	3–0 / 3
	MCH-3I5	Research Methodology (Inorganic)	Inorganic (RM)	4–0 / 4
	MCH-3IL	Inorganic Chemistry Lab–III	Practical	0–16 / 8
			Total L–P/Credits in Semester III for Inorganic Branch	**16–16/24**

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Sem	Paper Code	Course Title	Paper Type	L–P / Credits (UE+IA)
				Organic Branch Special (Spl.) Papers
III	MCH-3O1	Methods in Organic Synthesis	Organic Spl. (DSE)	3–0 / 3
	MCH-3O2	Rearrangement, named reactions and organomettalics	Organic Spl. (DSE)	3–0 / 3
	MCH-3O3	Heterocyclic Chemistry & Disconnection Approach	Organic Spl. (DSE)	3–0 / 3
	MCH-3O4	Bioorganic & biochemical reactions	Organic Spl. (DSE)	3–0 / 3
	MCH-3O5	Research Methodology (Organic Branch)	Organic (RM)	4–0 / 4
	MCH-3OL	Organic Chemistry Lab–III	Practical	0–16 / 8
			Total L–P/Credits in Semester III for Organic Branch	**16–16/24**
				Physical Branch Special Papers
III	MCH-3P1	Advanced Statistical Mechanics	Physical Spl. (DSE)	3–0 / 3
	MCH-3P2	Advanced Quantum Chemistry	Physical Spl. (DSE)	3–0 / 3
	MCH-3P3	Advanced Chemical Kinetics	Physical Spl. (DSE)	3–0 / 3
	MCH-3P4	Advanced Solid State Chemistry	Physical Spl.(DSE)	3–0 / 3
	MCH-3P5	Research Methodology (Physical Branch)	Physical (RM)	4–0 / 4
	MCH-3PL	Physical Chemistry Lab–III	Practical	0–16 / 8
			Total L–P/Credits in Semester III for Physical Branch	**16–16/24**
				Material Branch Special (Spl.) Papers
III	MCH-3M1	Polymer Chemistry and Macromolecular Architecture	Materials Spl. (DSE)	3–0 / 3
	MCH-3M2	Nanomaterials: Synthesis, Properties and Applications	Materials Spl. (DSE)	3–0 / 3
	MCH-3M3	Hybrid Materials and Computational Frontiers	Materials Spl. (DSE)	3–0 / 3
	MCH-3M4	Materials for Energy Conversion and Storage	Materials Spl. (DSE)	3–0 / 3
	MCH-3M5	Research Methodology (Material Branch)	Materials (RM)	4–0 / 4
	MCH-3ML	Material Chemistry Lab–III	Practical	0–16 / 8
			Total L–P/Credits in Semester III for Material Branch	**16–16/24**
				Inorganic Branch Special (Spl.) Papers
IV	MCH-4I1	Advanced Inorganic Spectroscopy	Inorganic Spl. (DSE)	2–0 / 2
	MCH-4I2	Stereochemistry and Metal Ion Catalysis	Inorganic Spl. (DSE)	2–0 / 2
	MCH-4I3	Advanced Organometallic Catalysis Chemistry	Inorganic Spl. (DSE)	2–0 / 2
	MCH-4I4	Comprehensive Bio-inorganic Chemistry-II	Inorganic Spl. (DSE)	2–0 / 2
	MCH-491	Project / Dissertation (Thesis + Viva)	Project (RC)	0–20 / 10
			Total L–P/Credits in Semester IV for Inorganic Branch	**8–20/18**
				Organic Branch Special (Spl.) Papers
IV	MCH-4O1	Medicinal Chemistry	Organic Spl. (DSE)	2–0 / 2
	MCH-4O2	Advanced Methods in Organic Synthesis	Organic Spl. (DSE)	2–0 / 2
	MCH-4O3	Natural Products and Structural Elucidation	Organic Spl. (DSE)	2–0 / 2
	MCH-4O4	Organic spectroscopy	Organic Spl. (DSE)	2–0 / 2
	MCH-491	Project / Dissertation (Thesis + Viva)	Project (RC)	0–20 / 10
			Total L–P/Credits in Semester IV for Organic Branch	**8–20/18**
				Physical Branch Special (Spl.) Papers

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Sem	Paper Code	Course Title	Paper Type	L–P / Credits (UE+IA)
IV	MCH-4P1	Non-Equilibrium Statistical Mechanics and Biophysical Systems	Physical Spl. (DSE)	2–0 / 2
	MCH-4P2	Advanced Molecular Spectroscopy	Physical Spl.	2–0 / 2
	MCH-4P3	Advanced Electrochemistry	Physical Spl. (DSE)	2–0 / 2
	MCH-4P4	Nanochemistry	Physical Spl. (DSE)	2–0 / 2
	MCH-491	Project / Dissertation (Thesis + Viva)	Project (RC)	0–20 / 10
			Total L–P/Credits in Semester IV for Physical Branch	**8–20/18**
				Material Branch Special (Spl.) Papers
IV	MCH-4M1	Functional Materials (Optical, Electronic and Magnetic)	Materials Spl. (DSE)	2–0 / 2
	MCH-4M2	Advanced Characterization Techniques	Materials Spl. (DSE)	2–0 / 2
	MCH-4M3	Basics in Crystallography	Materials Spl. (DSE)	2–0 / 2
	MCH-4M4	Emerging Materials and Device Applications	Materials Spl. (DSE)	2–0 / 2
	MCH-491	Project / Dissertation (Thesis + Viva)	Project (RC)	0–20 / 10
			Total L–P/Credits in Semester IV for Material Branch	**8–20/18**

MCH-101: Advanced Inorganic Chemistry-I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-101	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Metal Ligand Equilibria in Solution 15 L

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate Effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

Unit II: Magnetic Properties of Transition Metal Complexes 15 L

Magnetic properties of transition metal complexes and lanthanides, spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P., intra-molecular effects, anti- ferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria, anamolous magnetic moments, magnetic exchange coupling and spin Crossover.

Unit III: Inorganic Materials 15 L

Introduction to the solid state, metallic bond, band theory (zone model, brillouin zones, limitation of zone model): defects in solids, p-type and n-type, inorganic semiconductors (use in transistors, IC etc.), electrical, optical, magnetic and thermal properties of inorganic materials, superconductors, with special emphasis on the synthesis and structure of high temperature superconductors.

Essential Reading

1. Inczedy, J. *Analytical Applications of Complex Equilibria.* Halsted Press, New York, NY, 1976.
2. Hartley, F. R., Burgess, C., and Alcock, R. M. *Solution Equilibria.* Prentice–Hall, Europe, 1980.
3. Ringbom, A. *Complexation in Analytical Chemistry.* Wiley–Interscience, New York, 1963.
4. Carlin, R. L. *Magnetochemistry.* Springer–Verlag, Berlin, 1986.

MCH-101L: Inorganic Chemistry Lab-I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-101L	2	50 (UE=25, IA=25)	Practical

1. **Synthesis and Characterization of Complexes**

   Preparation of the following inorganic compounds and their characterization using IR, electronic spectra:

   (a) $VO(acac)_2$
   (b) Cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
   (c) $Na[Cr(NH_3)_2(SCN)_4]$
   (d) $[Co(PPh_3)_2Cl_2]$
   (e) $[Co(NH_3)_5]Cl_2$

2. **Quantitative Analysis**

   Separation and determination of the following two metal ion systems using volumetric and gravimetric methods:

   (a) Cu–Ni
   (b) Ni–Zn
   (c) Cu–Fe
   (d) Ba–Cu

3. **Spectrophotometric Determinations**

   (a) Determination of Ni by extractive spectrophotometric method.
   (b) Determination of Fe by Job's method of continuous variations.
   (c) Estimation of Fe in vitamin tablets.
   (d) Determination of Cr in solution.

Reference Books

1. W. G. Palmer, *Experimental Inorganic Chemistry*, Cambridge.
2. *Inorganic Synthesis*, McGraw Hill.
3. *Handbook of Preparative Inorganic Chemistry*, Vol. I and II, Academic Press.
4. W. W. Scott, *Standard Methods of Chemical Analysis*, Technical Press.
5. Vogel's *Qualitative Inorganic Analysis* (Revised), Orient Longman.
6. Vogel's *Textbook of Quantitative Inorganic Analysis* (Revised).

MCH-102: Sterochemistry & Reactive Intermediates

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-102	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Conformational & Configurational Isomerism 15 L

Conformations (sp^2 & sp^3) in open-chain (alkanes & alkenes) and cyclic systems (cyclopropane-to-cyclohexane, decalins, sugars, steroids, perhydroanthracene, perhydrophenanthrene). Effect of conformation on reactivity. Baeyer's strain theory. Fürst–Plattner (trans-diaxial) rule. Optical activity & chirality in one, two and more chiral centers including nitrogen, sulphur & phosphorus, resolution of racemic mixture. Different projection formulas. Relative & absolute configurations: D/L, R/S, & E/Z using CIP rules. Optical activity due to chiral axis: allenes, spiranes, hemispiranes, biphenyls, binaphthols & adamantane. Chirality due to helical shape & chiral plane. Optical purity: % enantiomeric excess (ee), & % diastereomeric excess (de). Topocity: Enantiotopic & diastereotopic atoms, groups & faces. Felkin–Anh, Hauk, Cieplak & Cornforth models, Cram's & Prelog's rules. Stereoselective and stereospecific reactions.

Unit II: Aromaticity & Principles of Reactivity 15 L

Alternant & non-alternant hydrocarbons; Frost circle diagrams and consequences of aromaticity; Hückel's, Craig's & Clair's rules, Peripheral, Homo-, Quasi-, Dual-, Y-type, Möbius-, Baird-type & ψ-aromaticity; Aromaticity in benzenoid & non-benzenoid systems including annulenes, fulvenes & fulvalenes. The HMO approach to compare the aromatic nature, NMR interpretation.

Transition state theory, Potential energy diagrams & Hammond's postulates, Curtin–Hammett principle, Winstein–Holness kinetics, Kinetic isotopic effects, Hammett's & Taft equations.

Unit III: Reactive Intermediates 15 L

Structure, preparation & properties of classical/nonclassical carbocations, neighboring group participation, Bredt's rule. Carbanions: Structure, preparation, and properties; Carbon free radicals: Stability and structure, generation and fate of free radicals, memory & captodative effects; radical-ions. Generation, structure and reactions of carbenes, nitrenes, nitrile ylides, benzynes intermediates. HSAB principle and its applications. Pinacol–Pinacolone, Wagner–Meerwein, Simmons–Smith, Reformatsky, abnormal Reimer–Tiemann, Doyle–Kirmse, Lombardo & Buchner reactions, Pfau–Plattner & Doering–Laflamme azulene synthesis, Grovenstein–Zimmerman, Wolff, Arndt–Eistert, Reed, Curtius, Hoffmann (isonitrile), Lossen, Schmidt, & Skattebøl rearrangements. Burton's reagent.

Books Suggested

1. Advanced Organic Chemistry; Jerry March, Fourth Edition, Wiley & Sons (2005).
2. Organic Chemistry; Paula Yurkanis Bruice, Third Edition, Pearson (2004).
3. Advanced Organic Chemistry; Francis A. Carey and Richard J. Sundberg, Part A & Part B.
4. Organic Reactions, Stereochemistry and Mechanisms; P. S. Kalsi, Fourth Edition, New Age International Publishers (2006).
5. Eliel, E. L. *Stereochemistry of Carbon Compounds.* Textbook Publishers, 2003.
6. Brückner, R. *Advanced Organic Chemistry.* Elsevier (2002).

7. *Theoretical and Physical Principles of Organic Reactivity* (1995), Addy Pross.
8. *Organic Chemistry* (Second Edition), by J. Clayden, N. Greeves, S. Warren.
9. *A Guidebook to Mechanism in Organic Chemistry*, Peter Sykes.
10. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, New Age International Publishers, 3rd Edition, 2011.
11. *Stereochemistry: Conformation and Mechanism*, P. S. Kalsi, New Age Publishers, Tenth Edition, 2019.
12. C. K. Ingold, *Structure and Mechanism in Organic Chemistry*, Cornell University Press.
13. Jack Hine, *Physical Organic Chemistry*, McGraw-Hill.

MCH-102L: Organic Chemistry Lab-I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-102L	2	50 (UE=25, IA=25)	Practical

1. **Purification Techniques (Demonstrations)**

   Purification of solvents and reagents using techniques such as crystallization, sublimation, fractional distillation, vacuum distillation, drying and storage of solvents, thin layer chromatography and column chromatography, etc.

2. **Separation of a Binary Mixture and Ternary Mixture of Organic Compounds and Identification of the Separated Components by Systematic Qualitative Organic Analysis**

   Mixtures of acids, bases, phenols and neutral compounds.

3. **Preparations of the Following Compounds**

   (i) Hippuric acid (Schotten–Baumann reaction).
   (ii) Dibenzylacetone (Claisen–Schmidt reaction).
   (iii) Acetophenone to oxime.
   (iv) Glucazone from glucose.
   (v) Hydantoin synthesis.
   (vi) Phenolphthalein.
   (vii) Fluorescein.
   (viii) Benzimidazole.
   (ix) Sorbic acid (Knoevenagel condensation).
   (x) BINOL from 2-Naphthol.
   (xi) Chalcone from acetophenone and benzaldehyde.

Suggested Books

1. Comprehensive Practical Organic Chemistry by V. K. Ahluwalia.
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST.
3. Advanced Practical Organic Chemistry by N. K. Vishnoi.
4. A Textbook of Practical Organic Chemistry by A. I. Vogel.

MCH–103: Mathematical Methods and Quantum Chemistry

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-103	3	100 (UE=60, IA=40)	Theory (Core)

Objective: To provide a rigorous foundation in the mathematical principles and quantum mechanical concepts essential for understanding atomic and molecular systems, while developing analytical and problem-solving skills required for advanced studies in spectroscopy, statistical mechanics, computational chemistry, and related areas of theoretical chemistry.

Unit–I: Mathematical Structure of Quantum Mechanics 10 L

Linear vector spaces, basis sets, inner products, orthogonality, normalization, and completeness. Linear operators and matrix representations; eigenvalue problems and diagonalization of Hermitian operators. Dirac bra–ket notation; operator algebra, commutators, projection operators, and closure relations. Change of representation and physical interpretation of operators in quantum mechanics.

Unit–II: Differential Equations and Mathematical Tools 10 L

Ordinary and partial differential equations in physical chemistry. Series solutions and Sturm–Liouville problems; orthogonality and completeness of eigenfunctions. Special functions arising in quantum mechanics: Hermite, Laguerre, and Legendre polynomials; recursion relations and Rodrigues formula. Fourier series and Fourier transforms with physical interpretation. Calculus of variations, Euler–Lagrange equations, Rayleigh–Ritz variational principle, and virial theorem with applications to the harmonic oscillator and hydrogen-like atoms.

Unit–III: Quantum Chemistry 25 L

Postulates of quantum mechanics and measurement theory. Linear, Hermitian, and unitary operators; compatible observables and uncertainty principle. Exactly solvable models: particle in one-, two-, and three-dimensional boxes; particle on a ring; degeneracy and symmetry considerations. Central force problems: angular momentum operators, eigenvalues and eigenfunctions; rigid rotor. Hydrogen atom: separation of variables, radial and angular wavefunctions, expectation values, and radial probability distributions. Introduction to approximation methods: time-independent non-degenerate perturbation theory and variational method; qualitative connection to chemical bonding.

Suggested References

- Atkins, P. W. and Friedman, R., *Molecular Quantum Mechanics*, Oxford University Press.
- McQuarrie, D. A., *Quantum Chemistry*, University Science Books.
- Levine, I. N., *Quantum Chemistry*, Pearson Education.
- Szabo, A. and Ostlund, N. S., *Modern Quantum Chemistry*, Dover.
- Arfken, G. B., Weber, H. J., and Harris, F. E., *Mathematical Methods for Physicists*, Academic Press.

MCH-103L: Physical Chemistry Lab–I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-103L	2	50 (UE=25, IA=25)	Practical

1. **Chemical Kinetics**
   (a) Determine the specific rate constant for the acid-catalysed hydrolysis of methyl acetate by the *Initial Rate Method*. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
   (b) Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
   (c) Study the saponification of ethyl acetate with sodium hydroxide volumetrically.

2. **Conductometry**
   (a) i. Determine the cell constant of the given conductivity cell at room temperature and study the equivalent conductance versus square root of concentration relationship of a strong electrolyte (KCl or NaCl) and a weak electrolyte (acetic acid).
   ii. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
   iii. Determine the equivalent conductance, degree of dissociation and dissociation constant (K_a) of acetic acid.
   (b) i. Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.
   ii. Study the conductometric titration of potassium sulphate solution versus barium chloride solution.
   (c) Study the conductometric titration of
   i. Acetic acid vs. sodium hydroxide.
   ii. Acetic acid vs. ammonium hydroxide.
   iii. HCl vs. NaOH.
   (d) Study the stepwise neutralization of a polybasic acid (e.g., oxalic acid, citric acid and succinic acid) by conductometric titration and explain the variation in the plots.

3. **Potentiometry**
   (a) Titrate hydrochloric acid and sodium hydroxide potentiometrically.
   (b) Determine the dissociation constant of acetic acid potentiometrically.
   (c) Titrate oxalic acid and sodium hydroxide potentiometrically.
   (d) Titrate a mixture of
   i. Strong and weak acids (hydrochloric and acetic acids).
   ii. Weak acid (acetic acid) and dibasic acid (oxalic acid).
   iii. Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide.
   iv. Titrate a solution of Mohr's salt against potassium permanganate potentiometrically.
   v. Titrate a solution of Mohr's salt against potassium dichromate potentiometrically.

Reference Book:

1. *Experiments in Physical Chemistry*, Garland, Nibler, and Shoemaker, McGraw-Hill.
2. *Practical Physical Chemistry*, B. Viswanathan and P.S. Raghavan, Viva Books.
3. *Advanced Practical Physical Chemistry*, J. B. Yadav, Goel Publishing House.
4. *Vogel's Textbook of Quantitative Chemical Analysis*, G. H. Jeffery et al., Pearson.
5. *Physical Chemistry: A Laboratory Manual*, Rajan Katoch, Universities Press.
6. *Experimental Physical Chemistry – A Laboratory Textbook*, V. D. Athawale and Parul Mathur, New Age International.

MCH–104: Materials Chemistry-I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-104	3	100 (UE = 60, IA = 40)	Theory (Core)

Objective: To provide a comprehensive understanding of solid-state structures, phase equilibria in multiphase materials, and the fundamental properties, thermodynamics, and characterization of polymers.

Unit I: Fundamentals of Solid-State Materials 15 L

General properties of solid-state materials, crystal lattice and unit cell, close packing of particles, different types of voids and close-packed structures, location of tetrahedral and octahedral voids in the cubical cell, packing efficiency of different types of cubic unit cells. Coordinate system and Miller planes. Band theory and structure factor. Crystal structure of simple ionic solids–NaCl, CaF_2, Na_2O, $CaTiO_3$ and ZnS. Bragg's equation, imperfections in solids and their effect on properties (only point defect), calculation of atomic radius and unit cell edge length in different crystal systems.

Unit II: Multiphase Materials 15 L

Solid solutions; Interstitial and Substitutional solid solutions; Complex solid solutions; Intermetallic compounds; Condensed phase rule; One component system–Si and Fe binary isomorphous system; Cu–Ni, Au–Cu, Hume-Rothery, solid solubility rule, Lever rule, Invariant phase equilibrium, eutectic formation (Pb–Sn), peritectic formation: Fe–Ni, Fe–C phase diagram, phase transformation: Fe–C alloys, ferrous and non-ferrous alloys.

Unit–III: Polymers and Polymeric Solutions 15 L

General characteristics, classification and examples of polymers; nomenclature of polymers; morphology of polymers; thermodynamics of polymer solutions; molecular weights and methods for measuring molecular weights; radius of gyration; optical activity in polymers; thermal analysis of polymers.

Essential Reading

1. Textbook of Polymer Science by F. W. Billmeyer.
2. Introduction to Polymers by R. J. Young and P. A. Lovell.
3. Polymer Chemistry by G. Challa.
4. Solid State Chemistry: An Introduction by Elaine A. Moore and Jennifer Readman.
5. Solid State Chemistry and its Applications by A. R. West.
6. Materials Science and Engineering by William D. Callister Jr. and David G. Rethwisch.

MCH-104L: Materials Chemistry Lab-l

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-104L	2	50 (UE=25, IA=25)	Practical

1. **Analysis of Steel and Brass Samples**
   1.1 To determine the percentage of manganese in the given sample of steel.
   1.2 To determine the percentage of phosphorus in the given sample of steel.
   1.3 To determine the percentage of copper in the given sample of brass.
   1.4 To determine the percentage of zinc in the given sample of brass.
   1.5 Data plotting: Using different tools.
2. **Synthesis of Polymers**
   2.1 To prepare polystyrene by the bulk polymerization method and report the yield and solubility.
   2.2 To determine the Molecular Weight of the prepared polystyrene by viscometry.
   2.3 To determine the Molecular Weight of commercial polystyrene by viscometry and compare the molecular weights of the prepared and commercial polystyrene.
3. **Synthesis of Nanomaterials**
   3.1 To synthesize different types of iron oxides:
      (i) Hematite (α-Fe_2O_3)
      (ii) Maghemite (γ-Fe_2O_3)
      (iii) Magnetite (Fe_3O_4)

Reference Books

1. Laboratory Manual prepared by the Teacher-in-Charge.

MCH–151: Molecular Spectroscopy

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH–151	3	100 (UE = 60, IA = 40)	Theory (Elective)

Unit I: Molecular Symmetry and Group Theory 10 L

Symmetry elements and symmetry operations; point groups; classification of molecules into point groups; matrix representation of symmetry operations; reducible and irreducible representations; Great Orthogonality Theorem (statement only); construction and properties of character tables; direct products; projection operator (introductory treatment); symmetry adapted linear combinations (SALCs); applications of group theory to molecular vibrations; determination of infrared and Raman active vibrational modes; selection rules for spectroscopic transitions; applications to molecular orbitals and hybridization.

Unit II: Rotational, Vibrational and Raman Spectroscopy 20 L

Electromagnetic radiation and interaction of radiation with matter; absorption, emission and scattering processes; transition probability; transition dipole moment; general selection rules based on symmetry ideas; spectral line width and line broadening; Boltzmann distribution; instrumentation for molecular spectroscopy; dispersive and Fourier Transform spectrometers.
Microwave spectroscopy: rigid and non-rigid rotor models; rotational spectra of diatomic molecules; rotational constants; Effect of isotopic substitution; Stark effect; determination of bond lengths; Classification of polyatomic molecules; Momental Ellipsoid; Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First and second order Stark effect.
Infrared spectroscopy: harmonic and anharmonic oscillator models; vibrational energy levels; Morse potential; derivation of selection rules; vibration-rotation spectra; P, Q and R branches; Breakdown of the Born-Oppenheimer approximation; normal modes of vibration; Normal coordinate analysis; Overtones and combination bands; group frequencies; Fourier Transform Infrared (FTIR) spectroscopy; applications.
Raman spectroscopy: classical and quantum theories; Rayleigh, Stokes and Anti-Stokes scattering; rotational and vibrational Raman spectra; polarization of Raman lines; mutual exclusion principle; FT-Raman spectroscopy; applications.

Unit III: Electronic Spectroscopy 15 L

Electronic spectroscopy: electronic transitions; selection rules; Franck–Condon principle; vibrational fine structure; solvent effects; charge-transfer spectra; ligand field spectra (introductory treatment); UV–Visible spectroscopy; instrumentation and applications.
Photophysical processes: fluorescence; phosphorescence; internal conversion; intersystem crossing; Jablonski diagram; Förster resonance energy transfer (FRET); Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.
Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects-viscosity, polarity, hydrogen bonding.
Modern spectroscopic techniques: Circular Dichroism (CD); Surface Enhanced Raman Spectroscopy (SERS); fluorescence anisotropy; time-resolved spectroscopy.

Suggested Books

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edition, Wiley.
2. P. K. Bhattacharya, *Group Theory and Its Chemical Applications*, Himalaya Publishing House.

3. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edition, Tata McGraw–Hill.
4. J. M. Hollas, *Modern Spectroscopy*, 4th Edition, Wiley.
5. P. F. Bernath, *Spectra of Atoms and Molecules*, 3rd Edition, Oxford University Press.
6. R. Kakkar, *Atomic and Molecular Spectroscopy: Basic Concepts and Applications*, Cambridge University Press.
7. D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, *Introduction to Spectroscopy*, 5th Edition, Cengage Learning.
8. P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, Oxford University Press.
9. I. N. Levine, *Quantum Chemistry*, 7th Edition, Pearson.
10. C. N. Banwell, *Essentials of Molecular Spectroscopy*, McGraw–Hill.

MCH-201: Advanced Inorganic Chemistry-II

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-201	3	100 (UE=60, IA=40)	Theory (Core)

Objective: The course deals with the electronic spectra of transition metal complexes, stereochemistry, bonding of main group compounds, and the fundamentals of metal clusters and cages.

Unit I: Electronic Spectra of Transition Metal Complexes 15 L

Spectroscopic ground states, correlation, crystal field theory and splitting in O_h, T_d, D_{4h} and C_{4v} systems. Orgel and Tanabe–Sugano diagrams for transition metal complexes (d^1–d^9). Calculation of Dq, B and β parameters, charge-transfer spectra, spectroscopic methods for assignment of absolute configuration in optically active metal chelates and their stereochemical information.

Unit II: Stereochemistry and Bonding in Main Group Compounds 15 L

VSEPR, Walsh diagrams (tri- and penta-atomic molecules), $d\pi$–$p\pi$ bonds, Bent's rule and energetic hybridization, simple reactions of covalently bonded molecules.

Unit III: Metal Clusters and Cages 15 L

Higher boranes, carboranes and metalloboranes, compounds with metal–metal multiple bonds, metal carbonyls and halide clusters.

Recommended Texts

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, Wiley–VCH, 1999.
2. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rd Edition, Oxford University Press.
3. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*.
4. Catherine E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*.

MCH-201L: Inorganic Chemistry Lab-l

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-201L	2	50 (UE=25, IA=25)	Practical

1. **Chromatography: Separation of Cations and Anions by**
   (a) Thin Layer Chromatography (TLC).
   (b) Column Chromatography – Ion Exchange.

2. **Synthesis and Characterization of Complexes**

   Synthesis of the following inorganic compounds and their characterization using IR and electronic spectra:

   (a) $[Co(Py)_2Cl_2]$
   (b) $[Ni(NH_3)_6]Cl_2$
   (c) Trans-bis(glycinato)copper(II)
   (d) Lanthanide complexes

3. **Spectrophotometric Determination**
   (a) Determination of Cu in a brass sample.
   (b) Determination of nitrate and nitrite in water sample.
   (c) Determination of Ca and Mg in milk and egg.
   (d) Determination of nickel in tea.

4. **Synthesis and Characterization of Nanomaterials**
   - Metal oxides and metal nanoparticles (NPs).

Reference Books

1. W. G. Palmer, *Experimental Inorganic Chemistry*, Cambridge.
2. *Inorganic Synthesis*, McGraw–Hill.
3. *Handbook of Preparative Inorganic Chemistry*, Vols. I and II, Academic Press.
4. Vogel's *Qualitative Inorganic Analysis* (Revised), Orient Longman.
5. Vogel's *Textbook of Quantitative Inorganic Analysis* (Revised), ELBS.

MCH-202: Pericyclic Reactions & Photochemistry

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-202	3	100 (UE=60, IA=40)	Theory (Core)

Objective: To provide a comprehensive understanding of pericyclic reactions, orbital symmetry, and photochemical transformations, with emphasis on their mechanisms, stereochemical outcomes, and synthetic applications.

Unit I: Electrocyclic Reactions 15 L

General pericyclic selection rules and their applications, frontier molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, 1,3,5,7-octatetraene and allyl systems. Electrocyclic reactions: conrotatory and disrotatory motions of $4n\pi$, $(4n+2)\pi$, and allyl systems. Correlation diagrams for 4π-electron and 6π-electron systems, torque selectivity (a special kind of selectivity in pericyclic reactions), and pericyclic reactions of ionic species including Nazarov, Mallory, Buchner and Bergman reactions.

Unit II: Cycloaddition and Sigmatropic Reactions 15 L

General orbital symmetry rules, [2+2], [4+2], [6+4], [8+2], [14+2], [3+2] (Criss–Cross), [4+3] (Katritzky) [5+2] and [2+2+2] cycloaddition reactions, cheletropic and cycloreversion reactions, 1,3-dipolar cycloadditions including click chemistry (Sharpless–Meldal triazole) and Gassman cycloaddition. Sigmatropic reactions: (1,3), (1,5), (1,7), (2,3), (3,3). Fluxional tautomerism, Alder–Ene and Conia–Ene reactions, Staudinger synthesis, Babler–Dauben Wittig, Mislow–Evans, Sommelet–Hauser, Mislow–Evans, Meisenheimer, Povarov, Bartoli, Cope, Claisen, Johnson–Claisen, Eschenmoser–Claisen, Ireland–Claisen reactions, etc.

Unit III: Photochemistry 15 L

Basics of photochemistry: Jablonski diagram, non-vertical energy transfer, isomerizations, and singlet oxygen reactions, photochemical additions (Ciamician photocoupling); reactions of 1,3-, 1,4- and 1,5-dienes: di-π-methane rearrangement. Photochemistry of carbonyl compounds: Norrish type I and II reactions (cyclic and acyclic), α,β-unsaturated ketones, β,γ-unsaturated ketones, cyclohexenones (conjugated), photochemistry of p-benzoquinones, Barton and Hoffman–Loeffler–Freytag reactions, Paternò–Büchi and De Mayo reactions, photooxidation and photoreduction, Photo Fries rearrangement of ethers and anilides.

Books Suggested

1. Carruthers, W. and Coldham, I., *Modern Methods of Organic Synthesis*, Cambridge University Press (2004).
2. Fleming, I., *Pericyclic Reactions*, Oxford Science Publications (1998).
3. Jagdamba Singh and Jaya Singh, *Photochemistry and Pericyclic Reactions*, New Academic Science, 2012.
4. Cox, A. and Camp, T., *Introduction to Photochemistry*, McGraw–Hill.
5. Turro, N. J. and Benjamin, W. A., *Molecular Photochemistry.*
6. Jonathan Clayden, Nick Greeves, and Stuart Warren, *Organic Chemistry*, Oxford University Press, 2014.

7. Gilchrist and Storr, *Organic Reactions and Orbital Symmetry*, Cambridge University Press, 2nd Edition, 1979.

8. Lowry and Richardson, *Mechanism and Theory in Organic Chemistry*, Harper Row Publishers, New York.

9. Charles Dupey and O. Chapman, *Molecular Reactions and Photochemistry*, Prentice Hall.

10. S. N. Mukharji, *Pericyclic Reactions*, McMillan.

11. T. H. Lowery and K. S. Richardson, *Mechanisms and Theory in Organic Chemistry*.

12. L. N. Ferguson, *The Modern Structural Theory in Organic Chemistry*, Prentice Hall.

13. H. O. House, *Modern Organic Reactions*, Benjamin.

14. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, Blackie Academic & Professional.

MCH-202L: Organic Chemistry Laboratory–II

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-202L	2	50 (UE=25, IA=25)	Practical

1. **Isolation of the Following**
   - (i) Extraction of casein and lactose from milk.
   - (ii) Isolation of caffeine from tea leaves.
2. **Preparations, Isolation and Characterizations**
   - (i) Mannich reaction.
   - (ii) Cannizzaro reaction.
   - (iii) Phthalimide from phthalic anhydride.
   - (iv) 2,3-Diphenylquinoxaline from benzil.
   - (v) Diethyl phthalate from phthalic anhydride.
   - (vi) Anthrone from anthracene.
   - (vii) Benzoic acid from benzamide.
   - (viii) Oxalic acid from sucrose.
   - (ix) Methyl orange from sulphanilic acid.
   - (x) 4-Iodonitrobenzene.
   - (xi) Benzhydrol from benzophenone.
   - (xii) Furfural from glucose.
3. **Melting Points, UV–Vis, and IR Spectra of Simple Compounds**

Books Suggested

1. *Practical Organic Chemistry*, Mann and Saunders.
2. *Comprehensive Practical Organic Chemistry*, V. K. Ahluwalia.
3. *Advanced Practical Organic Chemistry*, N. K. Vishnoi.
4. *A Textbook of Practical Organic Chemistry*, A. I. Vogel.

MCH-203: Irreversible & Statistical Thermodynamics

Semester	Paper No.	Credits	Total Marks	Paper Type
II	MCH-203	3	100 (UE = 60, IA = 40)	Theory (Core)

Course Objective

To develop a rigorous thermodynamic and statistical framework for understanding chemical systems away from equilibrium, with emphasis on entropy production, transport phenomena, fluctuations, and the statistical origin of macroscopic irreversibility. The course aims to bridge microscopic dynamics and macroscopic laws, thereby preparing students for advanced equilibrium and non-equilibrium statistical mechanics, stochastic processes, and modern applications in chemical and biological systems.

UNIT I: Mathematical & Statistical Foundations of Irreversibility 15 L

Probability theory for thermodynamics: Random variables and probability distributions. Moments and cumulants. Gaussian distribution and central limit theorem. Law of large numbers and the thermodynamic limit. Role of fluctuations in macroscopic systems.
Correlation functions and fluctuations: Time-independent correlation functions and their physical interpretation. Connection between fluctuations and response (conceptual introduction). Statistical origin of macroscopic stability.
Entropy from a statistical and information-theoretic viewpoint: Boltzmann entropy and Gibbs entropy. Qualitative connection with Shannon entropy. Entropy as a measure of disorder and missing information.
Conservation laws and balance equations: Continuity equation. Balance equations for mass, momentum, and energy. Relaxation processes and characteristic time scales.
Emergence of irreversibility: Coarse-graining and loss of microscopic information. Time-reversal invariance at the microscopic level versus macroscopic irreversibility. Conceptual preparation for non-equilibrium and stochastic descriptions (Langevin and master equations: qualitative motivation only).
Numericals: Gaussian probability calculations, fluctuation estimates, relaxation-time problems.

UNIT II: Irreversible Thermodynamics & Transport Phenomena 15 L

Irreversible Thermodynamics: Meaning and scope of irreversible thermodynamics; thermodynamic criteria for non-equilibrium states; phenomenological laws with emphasis on linear laws; Gibbs equation; Onsager's reciprocal relations; entropy production with specific examples; non-equilibrium stationary states; Prigogine's principle of maximum entropy production; coupled phenomena and their important applications.
Transport Phenomena: Diffusion coefficients; Fick's first and second laws of diffusion; relation between flux and viscosity; relation between diffusion coefficient and mean free path; relation between thermal conductivity, viscosity, and mean free path of a perfect gas; Einstein relation; Nernst–Einstein equation; Stokes–Einstein equation; and Einstein–Smoluchowski equation.
Numericals: entropy production, coupled flux calculations, Onsager coefficients.

UNIT III: Statistical Thermodynamics 15 L

Fundamentals: Concept of microstates and macrostates; statistical distributions with emphasis on binomial and multinomial distributions for non-degenerate and degenerate systems;

thermodynamic probability and most probable distribution; canonical and other statistical ensembles; statistical mechanics of systems of independent particles and its importance in chemistry. Stirling's approximation. Lagrange multipliers and derivation of distribution laws.
Quantum statistics: Boltzmann, Bose–Einstein, and Fermi–Dirac statistics. Comparison and physical significance. Applications to simple systems (qualitative). thermodynamic probability (W) for the three types of statistics; derivation of distribution laws (most probable distribution).
Applications to Ideal Gases: Molecular partition function and its factorization; evaluation of translational, rotational, and vibrational partition functions for monatomic, diatomic, and polyatomic gases; electronic and nuclear partition functions; calculation of thermodynamic properties of ideal gases in terms of partition functions; statistical definition of entropy; ortho- and para-hydrogen, statistical weights of ortho and para states, and symmetry number; calculation of equilibrium constants of gaseous reactions in terms of partition functions; perfect gas mixtures.
Numericals: entropy calculations, partition functions, fluctuation magnitudes, stability analysis.

Essential Reading

1. de Groot, S. R. and Mazur, P., *Non-Equilibrium Thermodynamics*, Dover Publications, New York, 1984 (Reprint of the original North-Holland edition, 1962).

2. Kondepudi, D. and Prigogine, I., *Modern Thermodynamics: From Heat Engines to Dissipative Structures*, John Wiley & Sons, Chichester, U.K., 1998.

3. McQuarrie, D. A. and Simon, J. D., *Physical Chemistry: A Molecular Approach*, University Science Books, Sausalito, California, 1997.

4. Atkins, P. and de Paula, J., *Physical Chemistry*, 10th Edition, Oxford University Press, Oxford, U.K., 2014.

5. Hill, T. L., *An Introduction to Statistical Thermodynamics*, Dover Publications, New York, 1986 (Unabridged republication of the 1960 edition).

6. McQuarrie, D. A., *Statistical Mechanics*, University Science Books, Sausalito, California, 2000.

MCH-203L: Physical Chemistry Lab–I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-203L	2	50 (UE=25, IA=25)	Practical

1. **Chemical Kinetics**
   (a) Determine the specific reaction rate of the potassium persulphate–iodide reaction by the *Initial Rate Method*.
   (b) Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.
2. **Conductometry**
   (a) Study the conductometric titration of a mixture of a strong and weak acid.
   (b) Titrate a moderately strong acid (salicylic/mandelic acid) by the
      i. salt-lime method,
      ii. double alkali method.
   (c) Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
   (d) Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
   (e) Titrate magnesium sulphate against $BaCl_2$ and its reverse titration.
   (f) Estimate the concentration of each component of a mixture of $AgNO_3$ and HNO_3 by conductometric titration against NaOH.
   (g) Determine the degree of hydrolysis of aniline hydrochloride.
3. **Potentiometry**
   (a) Determine the solubility and solubility product of an insoluble salt, AgX (X = Cl, Br or I), potentiometrically.
   (b) Determine the mean activity coefficient ($\gamma_\pm$) of 0.01 M hydrochloric acid solution.
   (c) Titrate phosphoric acid potentiometrically against sodium hydroxide.
   (d) Find the composition of the zinc ferrocyanide complex by potentiometric titration.
   (e) Titrate potentiometrically solutions of
      i. KCl/KBr/KI;
      ii. mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
   (f) Titrate Fe^{2+} with Ce^{4+} potentiometrically.
   (g) Determine zinc in the presence of calcium by potentiometric titration.
   (h) Verify the Debye–Hückel theory through the solubility of ionic salts.

Reference Books

1. Harris, D. C. *Quantitative Chemical Analysis*, 6th Ed., W. H. Freeman & Co. (2002).
2. *Experiments in Physical Chemistry*, R.C. Das and B. Behera – Tata McGraw-Hill.
3. J.B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing House.

4. J.N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry, Vol. I – Physical*, S. Chand & Co.

5. N.G. Mukherjee, *Selected Experiments in Physical Chemistry*, J.N. Ghose & Sons.

6. J.C. Ghosh, *Experiments in Physical Chemistry*, Bharti Bhavan.

7. B.D. Khosla, V.C. Garg, Adarsh Khosla, *Senior Practical Physical Chemistry*, R. Chand & Co.

MCH-204: Material Chemistry-II

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-204	3	100 (UE=60, IA=40)	Theory (Core)

Objective: To develop an understanding of symmetry principles in solids, fundamentals of nuclear chemistry and composite materials, and the rheological behaviour and processing techniques of polymers.

Unit I: Symmetries in Solids 15 L

Elements of symmetry: Axis of symmetry, plane of symmetry, inversion center and roto-reflection; point groups: C_n, C_{nh}, D_{nh}, D_{nd} and spherical point groups; features of character tables and their applications.

Unit II: Nuclear Chemistry and Composite Materials 15 L

Nuclear chemistry: Nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.
Composite Materials: Definition, general characteristics and classification, matrix, fillers, types of matrix and fillers, division of composites based on filler reinforcement pattern, dispersion-strengthened composites, Al-based (SAP) and Ni-based fibrous composites, critical length of fibers, effect of reinforcement pattern of fillers on mechanical properties of fibrous composites, types of fillers.

Unit III: Polymer Rheology and Processing 15 L

Definition of rheology, geometry of deformation, Newtonian and non-Newtonian behaviours, measurement of rheological properties, free volume and packing density of polymers, stress–strain relationship, time-dependent fluid responses, viscoelastic properties, mechanical models of a viscoelastic material, stress relaxation, creep and relaxation behaviour of plastics.
Classification of polymer processing: Extrusion and extruders, calendaring, film blowing, injection molding, blow molding, rotational molding, transfer and compression molding, vacuum forming, reaction injection molding.

Recommended Texts

1. *Introduction to Polymer Chemistry*, Charles E. Carraher Jr.
2. *Modern Nuclear Chemistry*, Walter D. Loveland, David J. Morrissey, and Glenn T. Seaborg.
3. *The Mathematical Theory of Symmetry in Solids*, C. J. Bradley and A. P. Cracknell.
4. *Nuclear Chemistry*, Gregory Choppin, Jan-Olov Liljenzin, and Jan Rydberg.
5. *Chemical Applications of Group Theory*, F. A. Cotton.

MCH-204L: Material Chemistry Lab-I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-204L	2	50 (UE=25, IA=25)	Practical

1. To prepare polymethyl methacrylate by the bulk polymerization method and determine its % yield and solubility.
2. To prepare phenol–formaldehyde resins (resoles and novolak).
3. To prepare Al_2O_3 by the precipitation method and determine its density.
4. To study the phase equilibrium diagram of the Pb–Sn system by the direct cooling curve method.
5. To determine the porosity and density of a given ceramic cube.
6. To prepare a copolymer by the bulk method and determine its % yield and solubility.
7. To show the crystal geometries and secondary interactions using Mercury, Diamond and other software.
8. Hirshfeld surface analysis using crystallographic information files (CIFs).
9. Methods of preparation of single crystals of discrete molecules: Slow evaporation, vapor diffusion and layering.
10. Determination of packing in crystals using crystallographic information files (CIFs).

Reference Books

1. Laboratory manuals prepared by the Teacher-in-Charge.

MCH-251: Interpretative Spectroscopy

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-251	3	100 (UE=60, IA=40)	Theory (Elective)

Unit I: UV–Visible and IR Spectroscopy 15 L

Basics, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, aromatic and heterocycles, Fieser–Woodward rules for conjugated dienes and carbonyl compounds, and effect of solvent on electronic transitions. IR frequencies of alkanes, alkenes, alkynes, aromatic compounds, and for all other functional groups. Effects of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Applications of UV–visible and IR spectroscopy in organic chemistry.

Unit II: Nuclear Magnetic Resonance (NMR) Spectroscopy 15 L

Basic ideas about instrumentation, detailed ^{1}H-, ^{13}C-, ^{19}F-, ^{11}B- and ^{31}P-NMR spectra, nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin–spin interactions, factors influencing coupling constant J, spin decoupling, anisotropic effects in alkenes, alkynes, aldehydes and aromatic compounds. Interpretation of NMR spectra of simple compounds. Determination of structures of organic compounds using combined UV–Vis, IR, NMR and mass spectral data.

Unit III: Mass Spectrometry (MS) 15 L

Principles of mass spectrometry (instrumentation, operation and representation of spectra), ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, nitrogen rule, Stevenson's rule, effect of isotopes, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested

1. J. M. Hollas, *Modern Spectroscopy*, John Wiley & Sons (2004).
2. H. Windawi and F. L. Ho (Eds.), *Applied Electronic Spectroscopy for Chemical Analysis*, Wiley Interscience.
3. W. Kemp, *Organic Spectroscopy*, Palgrave.
4. R. V. Parish, *NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry*, Ellis Harwood.
5. D. L. Pavia *et al.*, *Introduction to Spectroscopy*, 5th Edition, Cengage Learning India, 2015.
6. Robert M. Silverstein, Francis X. Webster, David J. Kiemle and David L. Bryce, *Spectrometric Identification of Organic Compounds*, 8th Edition (2014).
7. Walker and Straw, *Spectroscopy*, Vols. I & II.
8. P. S. Kalsi, *Spectroscopy of Organic Compounds*, New Age International, 2007.
9. M. Balci, *Basic ^{1}H- and ^{13}C-NMR Spectroscopy*, Elsevier, 2005.

MCH-3I1: Chemical Applications of Group Theory

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3I1	3	100 (UE=60, IA=40)	Inorganic Special (DSE)

Objective: Introducing the Concepts of Group Theory and Its Applications

Unit I: Symmetry Elements, Symmetry Operations and Character Tables

Symmetry elements and symmetry operations; symmetry planes and reflection, inversion centre, proper axes and proper rotations, improper axes and improper rotations, identity. Products of symmetry operations. Symmetry operations as group elements (multiplication table). Symmetry point groups (Schoenflies notation). Classes of symmetry operations. Equivalent symmetry elements and atoms. Character tables for C_{2v} and C_{3v} point groups (construction not required). Reducible and irreducible representations; analysis of reducible representations. Simple applications of character tables.

Unit II: Symmetry Aspects of Molecular Vibrations

Introduction to molecular vibrations; symmetry of normal vibrations; determination of the symmetry species of normal modes (normal mode analysis of H_2O, CO_3^{2-} and N_2F_2 molecules). Contribution of particular internal coordinates to normal modes. Symmetry selection rules for fundamental vibrational transitions (qualitative treatment). Use of symmetry considerations to determine the number of infrared- and Raman-active vibrations (illustrated using SF_4).

Unit III: Symmetry Aspects of Hybrid Orbitals and Combination of Atomic Orbitals

Transformation properties of atomic orbitals. Hybrid orbitals for σ-bond formation in trigonal planar (BCl_3), tetrahedral (CH_4), square planar $[PtCl_4]^{2-}$ and trigonal bipyramidal (PF_5) molecules. Hybridization schemes for σ-bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems. Mathematical form of equivalent and non-equivalent hybrid orbitals. Trigonal planar sp^2 equivalent hybrids in BCl_3; tetrahedral sp^3 equivalent hybrid orbitals in CH_4; trigonal bipyramidal dsp^3 non-equivalent hybrid orbitals in PF_5.

Essential Reading

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edition, John Wiley & Sons.
2. L. H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw–Hill.
3. M. Orchin and H. H. Jaffé, *Symmetry, Orbitals and Spectra*, Wiley–Interscience.
4. R. S. Drago, *Physical Methods in Chemistry*, Saunders College Publishing.
5. G. M. Barrow, *Molecular Spectroscopy*, McGraw–Hill.

MCH-3I2: Advanced Inorganic Reaction Mechanism

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3I2	3	100 (UE=60, IA=40)	Inorganic Special (DSE)

Objective: Concepts of Advanced Inorganic Reaction Mechanisms

Unit I: Inorganic Reaction Mechanisms in Octahedral Complexes

Introduction to labile and inert octahedral complexes; interpretation of lability and inertness of transition metal complexes using Valence Bond Theory (VBT) and Crystal Field Theory (CFT); factors affecting the lability of complexes. Types of substitution reactions: nucleophilic or ligand substitution (S_N) and electrophilic or metal substitution (S_E) reactions. Mechanisms of nucleophilic substitution reactions in octahedral complexes: S_N1 or dissociative and S_N2 or associative (or displacement) mechanisms. Hydrolysis reactions: mechanisms of acid and base hydrolysis reactions of octahedral Co(III) amine complexes.

Unit II: Mechanism of Substitution Reactions in Square Planar Complexes

Mechanisms of substitution reactions in Pt(II) complexes; factors affecting the reactivity of square planar complexes; trans effect; theories of the trans effect: Grinberg's electrostatic polarization theory and the Chatt–Orgel π-bonding theory; application of the trans effect to the synthesis of complexes.

Unit III: Electron Transfer (Oxidation–Reduction) Reactions

Electron transfer reactions; mechanisms of one-electron transfer reactions: outer-sphere and inner-sphere mechanisms; two-electron transfer reactions: complementary and non-complementary reactions; mechanisms of two-electron transfer reactions.

Essential Reading

1. Basolo, F. and Pearson, R. G., *Mechanisms of Inorganic Reactions*, 2nd Edition, John Wiley & Sons.
2. Edwards, J. O., *Inorganic Reaction Mechanisms*, W. A. Benjamin.
3. Langford, C. H. and Gray, H. B., *Ligand Substitution Processes*, W. A. Benjamin.
4. Malik, W. U., Madan, R. D. and Tuli, G. D., *Selected Topics in Inorganic Chemistry*, S. Chand & Company.
5. Katakis, D. and Gordon, G., *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.

MCH-3I3: Advanced Organometallic Chemistry-I

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3I3	3	100 (UE=60, IA=40)	Inorganic Special (DSE)

Objective: Introduction to Organometallic Chemistry

Unit I: Introduction to Organometallics: Main Group, Transition Elements and Metal Carbonyls

Introduction and classification of organometallic complexes; IUPAC nomenclature for metal π-complexes; synthesis of organometallic complexes by direct synthesis, redistribution method, metal exchange, ligand exchange, addition reaction, cyclization, sigma–pi rearrangements and substitution methods. Importance of organometallic complexes as reagents, additives and catalysts. Structure, π-bonding and bonding modes of CO; synthesis of metal carbonyls; reactions of metal carbonyls; carbonyl anions, cations and hydrides; Collman's reagent; metal nitrosyls.

Unit II: Ligands: Alkenes, Alkynes, Alkyl and Aryl Groups with Higher Hapticity

Models of alkene and alkyne–metal bonding; Zeise's salt; bonding and structural stability of metal–alkene complexes; the concept of umpolung; Pauson–Khand reaction; cyclopentadienyl as ligand; metal sandwich compounds; ferrocene and its reactions; Schwartz's reagent and hydrozirconation; arene π-complexes and their reactions; cyclooctatetraene (COT) as ligand; neutral spectator ligands.

Unit III: Structure Elucidation and IR Spectroscopy of Organometallic Complexes

Vibrational spectra and their applications; study of complex compounds; factors controlling the character of vibrations of large molecules. Coordination of inorganic groups in metal π-complexes: coordination of sulphate ions, coordination of nitrate ions, cyanate and thiocyanate complexes; study of bridged ligands; coordination and changes in the vibrations of C–O bonds; coordination of alkenes and changes in vibrations of C=C bonds.

Books Suggested

1. Pearson, A. J., *Metallo-Organic Chemistry*, John Wiley & Sons, 1985.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L., *Inorganic Chemistry: Principles of Structure and Reactivity*, 5th Edition, HarperCollins, 2005.
3. Tsutsui, M., Levy, M. N., Nakamura, A., Ichikawa, K. and Mori, K., *Introduction to Metal π-Complex Chemistry*, Plenum Press, New York, 1970.
4. Mehrotra, R. C. and Singh, A., *Organometallic Chemistry*, Wiley Eastern Ltd., 2000.
5. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., *Advanced Inorganic Chemistry*, 6th Edition, John Wiley & Sons, 1999.

MCH-3I4: Advanced Bio-inorganic Chemistry-I

Semester	**Paper No.**	**Credits**	**Total Marks**	**Paper Type**
III	MCH-3I3	3	100 (UE=60, IA=40)	Inorganic Special (DSE)

Objective: Fundamentals in Bioinorganic Chemistry

Unit I: Metal Uptake, Metalloproteins and Enzymes

Biological ligands for metal ions: macrocycles, nucleobases, nucleotides and nucleic acids; coordination of metals by proteins; heme and non-heme proteins; hemocyanin and hemerythrin. Principles involved in and roles of various metal ions (Zn, Fe, Cu and Co); carboxypeptidase, carbonic anhydrase, alcohol dehydrogenase, zinc fingers, other gene regulatory zinc proteins, cobalamin and mutase activities of coenzyme B_{12}.

Unit II: Transport of Inorganic Molecules

Oxygen transport and storage through hemoglobin and myoglobin; alternative oxygen transport in lower organisms; photosynthesis: photochemistry, absorption spectra of photosynthetic pigments, photophosphorylation and energy conversion processes.

Unit III: Metal Storage and Biomineralization

Structure and function of iron–sulfur proteins, cytochromes, cytochrome P-450 and oxygen-transfer proteins; long-distance electron transfer; siderophores, phytosiderophores, hemosiderin and biomineralization; assembly of advanced materials such as calcium phosphate and calcium carbonate in biominerals.

Essential Reading

1. Lippard, S. J. and Berg, J. M., *Principles of Bioinorganic Chemistry*, University Science Books.
2. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S., *Bioinorganic Chemistry*, University Science Books.
3. Eichhorn, G. L. (Ed.), *Inorganic Biochemistry*, Vols. I and II, Elsevier.
4. Lippard, S. J., *Progress in Inorganic Chemistry*, Vols. 18 and 38, Wiley.
5. Huheey, J. E., Keiter, E. A. and Keiter, R. L., *Inorganic Chemistry: Principles of Structure and Reactivity*, 6th Edition, HarperCollins.

MCH-3I5: Research Methodology (Inorganic Branch)

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3I5	4	100 (UE=60, IA=40)	Theory (Inorganic (RM))

Unit I: Concept and Literature Collection and Laboratory Safety

Systematic collection and processing of scientific data; analysis of information for advancement of knowledge; collection, organization and evaluation of data; drawing scientific conclusions; investigation and experimentation aimed at the discovery and interpretation of facts; identification of new facts and practical applications of new or revised theories and laws; laboratory safety practices; handling and disposal of chemical and plastic wastes; precautionary measures for the maintenance of laboratory equipment.

Unit II: Experimental Methods

Formulation of research problems; stages of the research process; preparation of research design; synthesis and hydrothermal synthesis; crystal structure determination; Hirshfeld surface analysis; density functional theory (DFT) calculations; spectral analysis of NLO-active compounds; collection of experimental data; spectrophotometric and physicochemical determination; morphological studies; photocatalytic degradation of organic molecules.

Unit III: Data Interpretation and Result Discussion

Errors, precision and accuracy; arithmetic mean, standard deviation, variance and chi-square test; applications of curve fitting, straight-line fitting and interpolation in solving chemical problems; applications of commonly used computer software including ChemDraw, ChemOffice, Mercury, Origin, Microsoft Excel and other tools for physicochemical data analysis.

Unit IV: Dissemination of Research Findings

Presentation of research findings; elements of scientific research publications; seminar presentation; patent writing; research paper writing; journal impact factor, i10-index and h-index; peer-review process.

Essential Reading

1. K. Prathapan, *Research Methodology for Scientific Research*, Dreamtech Press, 2019.
2. R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, World Health Organization (WHO), 2009.
3. Ramesh Kumari, *Computers and Their Applications to Chemistry*, 2nd Edition, Narosa Publishing House, 2007.
4. K. Atkinson, *Elementary Numerical Analysis*, 2nd Edition, John Wiley & Sons, 2003.
5. R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, World Health Organization (WHO), 2009.

MCH-3IL: Inorganic Chemistry Lab–III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3IL	8	200 (UE=100, IA=100)	Practical

1. **Synthesis of Inorganic Compounds**

   Preparation of the following compounds and their characterization by IR, electronic spectra, Mössbauer spectroscopy, ESR and magnetic susceptibility measurements. Handling of air- and moisture-sensitive compounds involving vacuum-line techniques.

   (a) Synthesis and thermal analysis of Group 2 metal oxalate hydrates.
   (b) Synthesis of metal acetylacetonates; magnetic, IR and NMR studies.
   (c) Determination of magnetic moment of $Cu(acac)_2{\cdot}H_2O$.
   (d) Synthesis of cis- and trans-$[Co(en)_2Cl_2]$.
   (e) Synthesis of Copper(II) macrocyclic complex.

2. **Spectrophotometric Determination**

   (a) Determination of Mn/Cr/V in steel samples.
   (b) Determination of Mo/W/V/U by extractive spectrophotometric method.
   (c) Spectrophotometric determination of PO_4^{3-}, As(III) and As(V).
   (d) Determination of Zr–Alizarin Red-S complex by mole-ratio method.
   (e) Determination of Cu–ethylenediamine complex by slope-ratio method.

3. **Simultaneous Determination of Metals Using UV–Visible Spectroscopy**

   - Simultaneous determination of Cr and Mn in solution.

Reference Books

4. W. G. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press.
2. *Inorganic Syntheses*, McGraw–Hill.
3. W. L. Jolly, *Handbook of Preparative Inorganic Chemistry*, Vols. I & II, Academic Press.
4. W. W. Scott, *Standard Methods of Chemical Analysis*, Technical Press.
5. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Qualitative Inorganic Analysis*, Revised Edition, Orient Longman.
6. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis*, Revised Edition.

MCH-3O1: Methods in Organic Synthesis

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3O1	3	100 (UE=60, IA=40)	Organic Special (DSE)

Unit I: Formation of C–C Single Bonds

Generation of thermodynamic and kinetic enolates and their applications in chiral synthesis; alkylation of enolates and enamines; silyl enol ethers; conjugate addition reactions of enolates and enamines (Stork enamine acylation/alkylation); Michael addition; Evans' and Mukaiyama aldol reactions; Narasaka–Prasad, Evans–Saksena and Evans–Tishchenko reactions; Baylis–Hillman reaction; Robinson, Danheiser and Hauser annulations; organoboron chemistry; cyclization reactions (Prins, Blanc and Johnson polyene cyclizations); organoboron chemistry and Baldwin's rules.

Unit II: Formation of C–C Double Bonds

Phosphorous and sulphur ylides: preparation and applications in organic synthesis. Role of silicon in organic synthesis: origin and consequence of α- and β-effects. Formation of alkenes using Wittig, Horner–Wadsworth–Emmons, Still–Gennari, Shapiro, Bamford–Stevens, Julia, Peterson, Kauffmann, Eastwood, Corey–Winter, McMurry, Takai, Taylor–Ireland, Martin's sulfurane, Burgess and Ramberg–Bäcklund olefinations. Alkene formation using Tebbe's, Petasis, Lombardo, Nysted and involving chromium-based reagents. Corey–Chaykovsky and Arbuzov reactions.

Unit III: Oxidation & Reduction

Oxidation of hydrocarbons: SeO_2, DDQ, Etard's and related reactions, Prevost and Woodward dihydroxylation, Sharpless asymmetric and Jacobsen's epoxidations, dihydroxylation and amino-hydroxylation. Palladium-catalyzed oxidation of alkenes.

Oxidation of alcohols: chromium reagents; oxidation via alkoxysulfonium salts (DCC); Swern oxidation; MnO_2, PCC, Jones reagent, Collins reagent; other metal-based oxidants (Ag_2CO_3, RuO_4 and $Tl(NO_3)_3$); oxidative cleavage of C–C bonds.

Catalytic hydrogenation of alkenes, alkynes, aromatic compounds, nitriles, oximes and nitro compounds. Heterogeneous and homogeneous catalysis. Reduction of carbonyl compounds (Wolff–Kishner's), aromatic compounds (Birch reduction), alkynes (cis- and trans-alkenes) and conjugated dienes. Hydride transfer reagents: aluminium alkoxides (MPV reduction), $LiAlH_4$, $NaBH_4$, $NaBH_3CN$, DIBAL–H; reductions with diimides and trialkyl tin hydrides; CBS, Noyori, Midland and enzymatic reductions. Borch, Caglioti and Leuckart–Wallach reductive aminations. Alkynes (Chan–Lam alkynylation) and conjugated dienes. Hydride transfer reagents: aluminium alkoxides (MPV reduction), $LiAlH_4$, $NaBH_4$, $NaBH_3CN$, DIBAL–H; reductions with diimides and trialkyl tin hydrides; CBS, Noyori, Midland and enzymatic reductions. Borch, Caglioti and Leuckart–Wallach reductive aminations.

Books Recommended

1. Smith, M. B. and March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 6th Edition, John Wiley & Sons, 2007.

2. Carey, F. A. and Sundberg, R. J., *Advanced Organic Chemistry*, Parts A & B, Plenum Press, U.S.A., 2004.

3. Carruthers, W. and Coldham, I., *Modern Methods of Organic Synthesis*, Cambridge University Press, 2004.

4. Zweifel, G. and Nantz, M. H., *Modern Organic Synthesis: An Introduction*, W. H. Freeman and Company, 2006.
5. Brückner, R., *Advanced Organic Chemistry: Reaction Mechanisms*, Elsevier, 2002.
6. Clayden, J., Greeves, N., Warren, S. and Wothers, P., *Organic Chemistry*, Oxford University Press, 2001.
7. Lowry, T. H. and Richardson, K. S., *Mechanism and Theory in Organic Chemistry*, Addison–Wesley Educational Publishers, Inc., 1981.
8. Lowry, T. H. and Richardson, K. S., *Mechanism and Theory in Organic Chemistry*, Harper & Row Publishers, New York.
9. House, H. O., *Modern Synthetic Reactions*, 2nd Edition, W. A. Benjamin, Inc., Menlo Park, California, 1972.
10. Brown, H. C., Kramer, G. W., Levy, A. B. and Midland, M. M., *Organic Syntheses via Boranes*, John Wiley & Sons, New York, 1975.

MCH-3O2: Rearrangement, named reactions and organomettalics

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3O2	3	100 (UE=60, IA=40)	Organic Special (DSE)

Unit I: Rearrangements and Fragmentations

General mechanistic considerations: nature of migration, migratory aptitude, memory effects, cationotropic and anionotropic rearrangements. Rearrangements involving electron-deficient carbon, nitrogen and oxygen. A detailed mechanistic study of the following: Kasha–Kiskii, Payne, Beckmann, Pummerer, Neber, Ciamician–Dennstedt, Boekelheide, Rupe and Meyer–Schuster's, Colvin, Saytzeff–Gilbert, Ohira–Bestmann, Fritsch–Buttenberg–Wiechell, Dakin, Stevens, Tiffeneau–Demjanov, Dienone–Phenol, Benzilic acid, Favorskii, Perkin, Brook, Smiles, Overman, Carroll, Plancher, Julia, Kornblum–DeLaMare, von Richter, Stieglitz, Achmatowicz, Amadori glucosamine, Black, Cargill, Chan, Chapman, Cloke–Wilson, Ferrier, Gabriel–Heine, Iocis, Meinwald, Aton, Walk, Newman–Kwart and Cornforth rearrangements. Aromatic rearrangements.
Basics of fragmentations: Grob, Eschenmoser, Wharton, Beckmann, Hanesian–Hullar, Hock, Marshall, Bernet–Vasella, Haller–Bauer, McDonald and Pummerer fragmentations.

Unit II: Strategic Applications of Named Reactions

Appel, Mitsunobu, Corey–Fuchs, Henry, Reigitz, Nef, Forster, Staudinger, Ritter, Koch–Haaf, Kulinkovich, Alkyne–zipper, Sakurai (Luche zinc allylation), Blanc, Dutta–Wormald, Schöll, Bergman (Myers–Saito and Moore), Mannich (list asymmetric Mannich), Betti, Bergini, Kabachnik–Fields, Ugi, Passerini, Smith–Tietze, Frankel–Shausaic, Chugaev, Delépine and Barton–Kellogg reactions.
Barton deoxygenation, deamination and decarboxylation; Duff, Sommelet, Bouveault, Bodroux–Chichibabin, Rieche, Vilsmeier–Haack and McFadyen–Stevens formylations; Benzoin, Stetter, Rubottom, Davis, Weiss–Cook, Hafner azulene, Weinreb and Haajos–Parrish ketone synthesis; Crabbe and Myers allene synthesis; Stobbe, Mills, Grieco, Pechmann and acyloin condensations; Yamaguchi, Corey–Nicolaou, Steglich, Yamamoto and Mukaiyama macrolactonizations.

Unit III: Organometallics in Organic Synthesis

Basics of organometallic chemistry; hapticity (η); 18-electron rule; Davies–Green–Mingos (DGM) and Wade rules; metal clusters; sandwich compounds; fluxional molecules; structure–bonding in metal–alkyls, aryls, allyls and cyclopentadienyl compounds; oxidative addition, reductive elimination, insertion, transmetallation, ortho- and cyclometallation, and agostic interactions.
Catalysis: turnover number (TON), turnover frequency (TOF), hydroformylation, hydrogenation, Monsanto and Cativa acetic acid process, Wilkinson's catalyst, Ziegler–Natta catalyst, Ziese's salt, metathesis, Wacker process. Pauson–Khand (Oppolzer cyclopentenone synthesis), Tsuji–Trost allylation, Nicholas, Buchwald–Hartwig, Petasis, Barluenga, Schwartz reaction; coupling reactions: A^3, Heck, Suzuki, Stille, Stille–Kelly, Sonogashira, Fukuyama, Hiyama, Negishi, Kumada, Chan–Lam, Castro–Stephens, Glaser, Eginton, Hay, Kochi–Fürstner, Nozaki–Hiyama–Kishi, Hegedus, Mori–Ban, Larock and other metal-catalyzed reactions (e.g., Fischer–indole, Michaelis–Arbuzov, Cacchi etc.).

Books Suggested

1. Kurti, L. and Czakó, B., *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press, 2004.

2. Carruthers, W. and Coldham, I., *Modern Methods of Organic Synthesis*, Cambridge University Press, 2004.
3. Zweifel, G. and Nantz, M. H., *Modern Organic Synthesis: An Introduction*, W. H. Freeman and Company, 2006.
4. Kumar, J., *Organometallic and Bioinorganic Chemistry*, Pragati Prakashan.
5. Mehrotra, R. C. and Singh, A., *Organometallic Chemistry*, Wiley Eastern Ltd., 2000.
6. Jenkins, P. R., *Organometallic Reagents in Synthesis*, Oxford Science Publications, Oxford, 1992.
7. Swan, J. M. and Black, D. C., *Organometallics in Organic Synthesis*, Chapman & Hall.
8. Gupta, B. D. and Elias, A. J., *Basic Organometallic Chemistry*, 2nd Edition, Universities Press (India) Pvt. Ltd., Hyderabad, 2013.
9. Smith, M. B., *Organic Synthesis*, McGraw–Hill Inc., New York, 1995.
10. Li, J. J., *Name Reactions*, 3rd Edition, Springer, 2003.
11. Bindra, J. S. and Bindra, R., *Creativity in Organic Synthesis*.
12. Jenkins, P. R., *Organometallic Reagents in Synthesis*.

MCH-3O3: Heterocyclic Chemistry & Disconnection Approach

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3O2	3	100 (UE=60, IA=40)	Organic Special (DSE)

Unit I: Retrosynthetic Analysis

The basis of retrosynthetic analysis and terminologies; synthons and synthetic equivalents (formyl/acyl anion, enolate, homoenolate, conjunctive species, linchpin strategy and other related species) and concept of umpolung. One-group (alcohol, carbonyl compounds, olefins and acids) and two-group (β-hydroxy, α,β-unsaturated carbonyl, 1,3-dicarbonyl and 1,5-dicarbonyl compounds) disconnections; implications of transforming substrate/precursor, functional group, mechanism, stereochemical, enantiodivergent and enantioconvergent based strategies and approaches. Synthesis of molecules by disconnection approach. Diverse functional group transformations. Protection and deprotection strategy.

Unit II: Three- to Five-Membered Heterocycles

Nomenclature of heterocyclic compounds; structure, preparation and reactivity of three- to five-membered heterocyclic compounds including diaziridines (Darzens, Charette, Julia, Payne and Prilezhaev), aziridines (Hassner, Hoch–Campbell, Scheiner, Wenker and Blum), oxiranes, azetidines, oxetanes, pyrroles (Paal–Knorr, Knorr, Barton–Zard, Piloty–Robinson, Clauson–Kaas, Hantzsch, Hinsberg, van Leusen and Trofimov), thiophene (Paal–Knorr, Paalmann, Fiesselmann, Gewald and Hinsberg), furan (Fiest–Benary, Paal–Knorr, butadiene oxidation and from allenyl ketones), imidazole (Debus–Radziszewski, van Leusen, Wallach and Marckwald), pyrazole, oxazole (Japp and Fischer) and thiazole (Hantzsch, Cook–Heilbron and modified Gewald).

Unit III: Six-Membered and Fused Heterocyclic Systems

Nomenclature, preparation and reactions of pyridine (Boger, Bohlmann–Rahtz, Chichibabin, Guareski–Thorpe, Hantzsch, Katritzky and Kröhnke), quinoline (Beyer, Combes, Conrad–Limpach, Döbner–Miller, Friedländer, Gould–Jacobs, Riehm, Knoorr, Meth–Cohn, Niementowski and Skraup), isoquinoline (Bischler–Napieralski, Brückner, Schlittler–Müller, Pictet–Gams and Pomeranz–Fritsch), indole (Fischer, Bartoli, Reissert, Madelung, Cadogan, Nenitzescu, Bischler–Möhlau, Castro and Fukuyama), carbazole (Bucherer, Graebe–Ullmann, Borche–Dreschel, Cadogan and Knölker), benzofuran and benzothiophene. Dihydropyridine, Biginelli, Chichibabin and Pictet–Spengler reactions.

Books Recommended

1. Warren, S. and Wyatt, P., *Organic Synthesis: The Disconnection Approach*, 2nd Edition, John Wiley & Sons, 2012.
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P., *Organic Chemistry*, Oxford University Press, Oxford, 2001.
3. Greene, T. W. and Wuts, P. G. M., *Protective Groups in Organic Synthesis*, John Wiley & Sons.
4. Gilchrist, T. L., *Heterocyclic Chemistry*, 3rd Edition, Addison–Wesley Longman Ltd., England, 1997.
5. Bansal, R. K., *Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms*, 3rd Edition, New Age International Publishers, New Delhi, 1999.
6. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin, V. V., *Handbook of Heterocyclic Chemistry*, 3rd Edition, Elsevier, Oxford, U.K., 2010.

7. Joule, J. A. and Mills, K., *Heterocyclic Chemistry*, 4th Edition, Blackwell Publishing, Indian Reprint, 2004.
8. Gupta, R. R., Kumar, M. and Gupta, V., *Heterocyclic Chemistry*, Vols. I–III, 1st Edition, Springer–Verlag, Berlin–Heidelberg, 2005.
9. Davies, D. T., *Aromatic Heterocyclic Chemistry*, Oxford University Press, 1992.
10. Corey, E. J. and Cheng, X.-M., *The Logic of Chemical Synthesis*, John Wiley & Sons.
11. Norman, R. O. C., *Principles of Organic Synthesis*, Chapman & Hall.
12. Bindra, J. S. and Bindra, R., *Creativity in Organic Synthesis.*
13. Katritzky, A. R., *Heterocyclic Chemistry.*
14. Parikh, A., *The Essence of Heterocyclic Chemistry*, 1st Edition, New Age International Publishers, 2010.

MCH-3O4: Bioorganic & biochemical reactions

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3O2	3	100 (UE=60, IA=40)	Organic Special (DSE)

Unit I: Bioorganic Chemistry of Amino Acids, Peptides, Sugars and Nucleic Acids

Overview of bioorganic chemistry; historical connections between organic and bioorganic chemistry. Basic concepts, physicochemical properties and synthesis of natural and unnatural amino acids (Strecker, Beller, Bucherer–Bergs, Darsapsky, Erlenmeyer, Ninhydrin, Gabriel and HVZ reactions). Charge, isoelectric point and synthesis of peptides (Woodward, Fischer, Yamada, and N/C-protecting groups). Sugars: classification, protecting group tactics, glycosylations and oligosaccharide formations. Basic ideas about nucleic acids, lipids and fatty acids.

Unit II: Bioorganic Chemistry of Proteins and Metalloporphyrins

Basic concepts of proteins, photosystems, porphyrins, heme and non-heme proteins. Oxygen-activating proteins (cytochrome P-450, cytochrome *c*); electron transport proteins (cytochromes, blue-copper and iron–sulfur proteins). Structure and functions of haemoglobin, myoglobin, hemocyanin, plastocyanin, hemoerythrin, hemosiderin, ferritin, transferrin, cyanocobalamin and chlorophylls. Role of alkali and alkaline earth metal ions in biological systems. Na^+/K^+-pump, ionophores and crown ethers.

Unit III: Biomolecular Catalysis

Introduction to biomolecular catalysis; role of weak interactions in catalysis; preliminary ideas about enzymes, cofactors, coenzymes (vitamin B_{12}), apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. Factors affecting the rate of enzyme-catalyzed reactions; enzyme inhibitors; enzyme browning. Biological significance and mechanistic aspects of carboxypeptidase, carbonic anhydrase, blue oxidases, non-blue oxidases, superoxide dismutase, peroxidase, lipases, proteases, alcohol dehydrogenase, chymotrypsin, hydrogenase, nitrogenase, cyanocobalamin and urease. Some important organic reactions in biological pathways.

Books Suggested

1. Lehninger, A. L., Nelson, D. L. and Cox, M. M., *Lehninger Principles of Biochemistry*, 5th Edition, W. H. Freeman, 2008.
2. Dugas, H., *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, 3rd Edition, Springer, 1996.
3. Davies, G. B. and Fairbanks, A. J., *Carbohydrate Chemistry*, 1st Edition, Oxford University Press, 2002.
4. Doonan, S., *Nucleic Acids*, 1st Edition, RSC Publishing, London, 2000.
5. Silverman, R. B., *The Organic Chemistry of Enzyme-Catalyzed Reactions*, Revised Edition, Academic Press, 2002.
6. Vranken, D. L. and Weiss, G. A., *Introduction to Bioorganic Chemistry and Chemical Biology*, 1st Edition, Garland Science, 2012.
7. McMurry, J. and Begley, T. P., *The Organic Chemistry of Biological Pathways*, 2nd Edition, W. H. Freeman, 2015.
8. Nelson, D. L. and Cox, M. M., *Lehninger Principles of Biochemistry*, 7th Edition, W. H. Freeman, 2017.

9. Frey, P. A. and Hegeman, A. D., *Enzymatic Reaction Mechanisms*, 1st Edition, Oxford University Press, USA, 2007.

10. Levy, D. E. and Fügedi, P., *The Organic Chemistry of Sugars*, CRC Press, 2006.

11. Lloyd–Williams, P., Albericio, F. and Giralt, E., *Chemical Approaches to the Synthesis of Peptides and Proteins*, 1st Edition, CRC Press, Boca Raton, 1997.

12. Doonan, S., *Peptides and Proteins*, 1st Edition, RSC Publishing, London, 2002.

MCH-3O5: Research Methodology (Organic Branch)

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3O5	4	100 (UE=60, IA=40)	Theory (Organic (RM))

Unit I: Fundamentals of Research Methodology and Scientific Literature (10L)

Introduction, objectives and significance of research; types of research: basic, applied and interdisciplinary; research process; identification of research problems and formulation of hypotheses; research design and planning; Good Laboratory Practices (GLP) and laboratory safety; primary, secondary and tertiary sources of scientific information; scientific journals, books and review articles; literature search using Google Scholar, SciFinder, Scopus, Web of Science and PubChem; search strategies: keywords, Boolean operators, citation searching; research metrics: Impact Factor, h-index, Citation Index, ORCID, Google Scholar Profile and ResearchGate.

Unit II: Experimental Methods in Organic Chemistry (10L)

Planning and execution of organic synthesis; selection of reagents, solvents and reaction conditions; principles of green chemistry in organic synthesis; reaction monitoring by Thin Layer Chromatography (TLC); purification techniques: recrystallization, distillation, solvent extraction and column chromatography; characterization techniques: UV–Visible spectroscopy, FTIR spectroscopy, ^{1}H and ^{13}C NMR spectroscopy, mass spectrometry; data recording, yield calculation, error analysis and interpretation of experimental results.

Unit III: Scientific Communication, Publication Ethics and Intellectual Property Rights (10L)

Scientific writing: research papers, review articles and dissertations; preparation of abstracts, posters and oral presentations; scientific referencing and bibliography; reference management software (Mendeley, Zotero); publication ethics and responsible conduct of research; plagiarism, fabrication, falsification and duplicate publication; authorship criteria and peer review; predatory journals; introduction to Intellectual Property Rights (IPR), patents, copyrights and technology transfer.

Unit IV: Statistical Methods and Computer Applications in Chemistry (10L)

Types of experimental data; data collection and processing; measures of central tendency and dispersion; error analysis; correlation and regression; hypothesis testing; Student's t-test, F-test, Chi-square test; basic ANOVA; graphical representation of data; applications of Microsoft Excel, Origin, ChemDraw and ChemOffice in chemical research.

Suggested Reading

1. D. C. Harris, *Quantitative Chemical Analysis*, 10th Edition, W. H. Freeman.
2. D. Harvey, *Modern Analytical Chemistry*, McGraw–Hill.
3. D. S. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th Edition, Cengage Learning.
4. J. M. Miller and J. C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, 7th Edition, Pearson.
5. D. C. Montgomery and G. C. Runger, *Applied Statistics and Probability for Engineers*, Wiley.
6. M. W. Beck, *Data Analysis for Chemistry: An Introductory Guide for Students and Laboratory Scientists*, Oxford University Press.

MCH-3OL: Organic Chemistry Lab–III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3OL	8	200 (UE=100, IA=100)	Practical

1. **Isolation of some important natural products.**
   (a) Isolation of piperine from black pepper.
   (b) Isolation of lycopene from tomatoes.
   (c) Isolation of eugenol from cloves.
   (d) Isolation of nicotine dipicrate from tobacco.
2. **Preparations, purification & characterizations: (one/two/three-stage).**
   (a) 7-Hydroxy-4-methyl coumarin from resorcinol.
   (b) Synthesis of Phenytoin.
   (c) 3-Methyl-1-phenyl-5-pyrazoline from phenyl hydrazine.
   (d) Benzoin → Benzil → Benzilic Acid.
   (e) Diels–Alder reaction of anthracene with maleic anhydride.
   (f) 1,2,3,4-Tetrahydrocarbazole from cyclohexanone & phenylhydrazine.
   (g) Benzophenone → Benzophenone oxime → Benzanilide (Beckmann).
   (h) Nitrobenzene → m-dinitrobenzene → m-nitroaniline → m-nitrophenol.
   (i) Phthalic anhydride → phthalimide → anthranilic acid.
   (j) Eosin from phthalic anhydride.
   (k) Succinic anhydride from succinic acid.
   (l) 3,4-Dihydro-1-hydroxy-4-oxophthalazine from phthalic anhydride.
   (m) Aniline from nitrobenzene.
   (n) Fries rearrangement: Phenyl acetate.
   (o) Anthranilic & Barbituric acids.
   (p) 2,4-Dihydroxyacetophenone.

Suggested Books

1. V. K. Ahluwalia, *Comprehensive Practical Organic Chemistry.*
2. *Monograph on Green Chemistry Laboratory Experiments*, Green Chemistry Task Force Committee, DST.
3. N. K. Vishnoi, *Advanced Practical Organic Chemistry.*
4. A. I. Vogel, *A Textbook of Practical Organic Chemistry.*

MCH-3P1: Advanced Statistical Mechanics

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3P1	3	100 (UE=60, IA=40)	Physical Special (DSE)

Course Objective

To develop a rigorous understanding of equilibrium statistical mechanics of interacting many-body systems, phase transitions, and polymeric matter, supplemented with essential mathematical and computational tools required for advanced statistical modeling in chemistry, soft matter, and materials science.

Unit I: Interacting Systems and Imperfect Gases 15 L

Classical many-particle systems and interaction potentials. Pair correlation function and radial distribution function. Equation of state of real gases. Virial expansion and virial coefficients. Mayer cluster expansion (conceptual introduction). Applications to real gases and simple liquids. Thermodynamic stability and compressibility relations.
Numericals: virial coefficients, compressibility factor, equation of state of real gases.

Unit II: Lattice Models, Phase Transitions and Critical Phenomena 15 L

Lattice models in statistical mechanics. Ising model: exact solution of one-dimensional Ising model and qualitative discussion of two-dimensional Ising model. Mean-field approximation and Bragg–Williams theory. Order parameter, symmetry breaking, and spontaneous magnetization. First- and second-order phase transitions. Thermodynamic potentials and phase stability. Landau theory of phase transitions. Introduction to critical phenomena and scaling laws (qualitative).
Numericals: magnetization, susceptibility, critical temperature, mean-field exponents.

Unit III: Statistical Mechanics of Polymer Systems 15 L

Polymers as many-body systems. Random walk and freely jointed chain models. End-to-end distance and radius of gyration. Gaussian chain model and configurational probability distribution. Entropic elasticity and force–extension relations. Ideal versus real polymer chains; excluded volume effects. Flory mean-field theory and scaling concepts. Thermodynamics of polymer solutions: Flory–Huggins theory. Introductory polymer dynamics: Rouse model (conceptual).
Numericals: mean-square end-to-end distance, radius of gyration, force–extension relations, Flory interaction parameter.

Essential Readings

1. Pathria, R. K. and Beale, P. D., *Statistical Mechanics*, 3rd ed., Elsevier.
2. Huang, K., *Statistical Mechanics*, 2nd ed., Wiley.
3. McQuarrie, D. A., *Statistical Mechanics*, University Science Books.
4. Chaikin, P. M. and Lubensky, T. C., *Principles of Condensed Matter Physics*, Cambridge University Press.
5. Rubinstein, M. and Colby, R. H., *Polymer Physics*, Oxford University Press.

MCH-3P2: Advanced Quantum Chemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3P2	3	100 (UE=60, IA=40)	Physical Special (DSE)

Objective: To provide a comprehensive understanding of exactly solvable quantum mechanical problems, approximate methods, molecular orbital theory, and density functional theory for applications in atomic, molecular, and computational chemistry.

Unit I: Some Exactly Solvable Problems 15 L

Review of postulates of quantum mechanics. Operators: Algebra, Hermitian operator, ladder-operator methods. The solution of the Schrödinger equation to some exactly solvable problems: systems viz. free particle, particle in a one-dimensional box, two- and three-dimensional box with infinite potential barrier, Jahn–Teller effect, particle with one and two finite potential barriers, quantum mechanical tunneling, the rigid rotor in two- and three-dimensional (particle on the surface of a sphere) and its extension to the hydrogen atom, one-dimensional harmonic oscillator.

Unit II: Approximate Methods 15 L

The variation theorem: linear variation principle. Time-independent perturbation theory (first-order and non-degenerate), second-order change of energy (non-degenerate). Applications of variation method and perturbation theory to the helium atom. Time-dependent perturbation theory. The Hartree–Fock self-consistent field method.

Unit III: Molecular Orbital Theory 15 L

Hybridization and valence molecular orbitals of H_2O, NH_3, and CH_4. Hückel molecular orbital (HMO) theory of conjugated hydrocarbon heteroatom systems, including heteroatoms. Delocalization energy, electron density, bond order. Application of HMO to hydrocarbons such as ethylene, butadiene, allyl and cyclopropenyl radical, benzene and their heteroatom analogues.
Density Functional Theory (DFT): Electron density, functionals, the Hohenberg–Kohn theorem, the Hohenberg–Kohn variational theorem, the Kohn–Sham (KS) method, the exchange–correlation energy functional, performing Kohn–Sham density functional calculations, hybrid functionals.

Books Recommended

1. P. W. Atkins and Ronald S. Friedman, *Quantum Chemistry*, 5th Edition, Prentice Hall, New Jersey (2000).
2. P. Engel and P. Reid, *Physical Chemistry*, Published by Pearson Education and Dorling Kindersley (India), 2006.
3. Donald A. McQuarrie, *Quantum Chemistry*, 2nd Edition, Oxford University Press, 1983.
4. A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw–Hill Publishing Company, New Delhi, 1994.
5. Irving Kaplan, *Quantum Chemistry*, Walter and Kimball, John Wiley & Sons Inc., Chapman & Hall Ltd., 1946.
6. David J. Griffiths, *Introduction to Quantum Chemistry*, 2nd Edition, Pearson Education International, 2005.
7. Peter Atkins and Julio de Paula, *Physical Chemistry*, 8th Edition, Oxford University Press.

MCH-3P3: Advanced Chemical Kinetics

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3P3	3	100 (UE=60, IA=40)	Physical Special (DSE)

Unit I: Statistical Theories of Kinetics 15 L

Collision theory. Collision cross section. Opacity function. Harpoon mechanism. Postulates and derivation of transition state theory. Potential energy surfaces. Thermodynamic formulation of transition state theory and its applications.
Unimolecular reaction rate theory: Lindemann–Hinshelwood mechanism. Rice–Ramsperger–Kassel (RRK) theory. Marcus refinement of RRK theory (RRKM).

Unit II: Complex Reactions 15 L

Chain reactions. Oscillatory reactions. Photochemical reactions.
Enzyme kinetics: Michaelis–Menten mechanism with single and double intermediates. King–Altman method for evaluation of rate equations. Enzyme-catalysed reactions and various types of inhibition.

Unit III: Kinetic Measurements 15 L

Introduction to kinetic measurements. Initiation methods. Kinetic systems: static systems, flow systems, and shock tubes.
Description of experimental techniques: flash photolysis and laser flash photolysis, absorption spectroscopy, laser photolysis and chemiluminescence, laser-induced fluorescence, photoionization techniques.
Treatment and analysis of kinetic data.

Essential Reading

1. Laidler, K. J., *Chemical Kinetics*, 3rd Edition, Harper & Row, 1987.
2. Wilkinson, L., *Chemical Kinetics*.
3. Pilling, M. J. and Seakins, P. W., *Reaction Kinetics*, Oxford University Press, Oxford, 1995.
4. Steinfeld, J. I., Francisco, J. S. and Hase, W. L., *Chemical Kinetics and Dynamics*, 2nd Edition, Prentice Hall, 1998.
5. Espenson, J. H., *Chemical Kinetics and Reaction Mechanisms*, 2nd Edition, McGraw–Hill, 1995.
6. Atkins, P. W. and de Paula, J., *Atkins' Physical Chemistry*, 8th Edition, Oxford University Press, 2006.
7. Upadhyay, S. K., *Chemical Kinetics and Reaction Dynamics*, Anamaya Publishers, New Delhi, 2006.
8. Steinfeld, J. I., Francisco, J. S. and Hase, W. L., *Chemical Kinetics and Dynamics*, 2nd Edition, Prentice Hall International, 1999.
9. Arnaut, L., Formosinho, S. and Burrows, H., *Chemical Kinetics: From Molecular Structure to Chemical Reactivity*, Elsevier.

MCH-3P4: Advanced Solid State CHemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
III	MCH-3P4	3	100 (UE=60, IA=40)	Physical Special (DSE)

Objective: To provide a comprehensive understanding of crystal structures, defects, non-stoichiometry, and the structural, electrical, magnetic, and electronic properties of solid-state materials.

Unit I: Chemistry of Solids **15 L**

Crystalline and amorphous solids, unit cell, summary of crystal lattices, reciprocal lattice, bonding and packing in crystals, lattice planes, symmetry elements, space lattice, glide planes, screw axis, point groups and notation of 32, 222, $mm2$ and mmm point groups, space groups and elucidation of representative point groups, viz. Monoclinic $C2$, Monoclinic $C2/m$, Orthorhombic $P222_1$ and Tetragonal $I4_1$.

Unit II: Crystal Defects and Non-Stoichiometry in Solids **15 L**

Perfect and imperfect crystals, intrinsic and extrinsic defects, point defects, line defects and plane defects, Schottky and Frenkel defects, thermodynamics of Schottky and Frenkel defect formation, F-, V- and H-colour centers, non-stoichiometry in solids and their mathematical calculations.

Unit III: Functional Properties of Solids **15 L**

(a) Electrical Properties: Dielectric materials, dielectric properties (dielectric constant and dielectric loss), dependence of dielectric properties on size, polarizability, concepts of ferroelectricity, pyroelectricity and piezoelectricity.

(b) Magnetic Properties: Classification of materials, line of force, effect of temperature, magnetic moment calculations, ferro-, ferri- and antiferromagnetic ordering, dependence of magnetic properties on size, magnetic domains and hysteresis.

(c) Electronic Properties: Metals, insulators, semiconductors and superconductors, density of states, origin of bands, E–k diagrams, bonding in solids, band theory, intrinsic and extrinsic semiconductors, p–n junction.

Essential Reading

1. Anthony R. West, *Solid State Chemistry and Its Applications*, John Wiley & Sons.
2. Lesley Smart and Elaine Moore, *Solid State Chemistry*, Chapman & Hall.
3. A. K. Cheetham and Peter Day, *Solid State Chemistry Techniques*, Oxford University Press.

Suggested Reading

1. C. N. R. Rao and J. Gopalakrishnan, *New Directions in Solid State Chemistry*, Cambridge University Press.
2. M. A. Shah and Tokeer Ahmad, *Nano Science & Technology*, I. K. International Pvt. Ltd., 2021.
3. H. V. Keer, *Principles of the Solid State*, New Age International Publishers.
4. D. K. Chakrabarty, *Solid State Chemistry*, New Age International Publishers.

MCH-3P5: Research Methodology (Physical Branch)

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3P5	4	100 (UE=60, IA=40)	Theory (Physical (RM))

Unit I: Molecular Modeling, Visualization & Scientific Data Analysis 10 L

Introduction to molecular modelling. Molecular mechanics and force fields; molecular geometry optimization; conformational analysis; molecular docking (introductory concepts).
Introduction to scientific software and data analysis tools: OriginPro, MATLAB, Python (NumPy, SciPy and Matplotlib), Microsoft Excel, Gnuplot and R (overview). Visualization and analysis using GaussView/Avogadro/VESTA etc. Quantum chemical calculations using Gaussian and ORCA (overview).
Linear and nonlinear curve fitting; interpolation and extrapolation; error bars and confidence intervals; histogram, box plot, contour plot and three-dimensional surface plot; residual analysis and goodness of fit. Preparation of publication-quality figures and tables; graphical abstract design; data reproducibility and FAIR data principles.

Unit II: Relaxation Kinetics 10 L

Theory of Chemical Relaxation; Relaxation Times in Two-Step Systems ; Relaxation Times in Common Multistep Systems ; Relaxation Amplitudes in Multistep Systems ; Evaluation of Relaxation Times from Experimental Relaxation Curves ; Experimental Techniques: Temperature-Jump, Pressure-Jump, Electric-Field-Jump, Concentration- Jump Methods, Stationary Electric Field method, Ultrasonics Techniques. Applications of Chemical Relaxation: Proton Transfer reactions, Neutralization Reactions, Protolysis and Hydrolysis reactions, the formation of Metal-Ion Complexes.

Unit III: Solution Chemistry 10 L

Volumetric studies of solutions: apparent molar volume, partial molar volume, transfer partial molar volume and their determination from density measurements; concentration dependence of apparent molar volume; Masson's equation; limiting partial molar properties and their significance; solute–solvent and solute–solute interactions.
Micellization studies: surfactants and critical micelle concentration (CMC); aggregation behaviour and thermodynamics of micellization; Gibbs free energy, enthalpy and entropy of micellization; effect of additives, salts, co-solvents and temperature on micellization; mixed micellization and regular solution theory.
Ultrasonic interferometric studies: principle and instrumentation of ultrasonic interferometer; determination of ultrasonic velocity in liquids and liquid mixtures; adiabatic compressibility, intermolecular free length, acoustic impedance, molar sound velocity and relaxation strength; effect of temperature and concentration on molecular interactions in liquid systems.

Unit IV: Characterization of Nanomaterials 10 L

Theory and instrumentation of X-ray diffractometer; structural elucidation using X-ray diffraction; Laue and powder diffraction methods; determination of crystallite size using X-ray line broadening studies (Scherrer equation); theory, instrumentation and applications of Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM); principle, theory and methodology of Dynamic Light Scattering (DLS) and Brunauer–Emmett–Teller (BET) surface area analysis.

Books Suggested

1. C. R. Kothari and G. Garg, *Research Methodology: Methods and Techniques*, 4th Edition, New Age International Publishers.
2. R. Kumar, *Research Methodology: A Step-by-Step Guide for Beginners*, 5th Edition, Sage Publications.
3. Relaxation Kinetics by Claude F. Bernasconi, Academic Press, New York, 1976
4. H. Strehlow and W. Knoche, *Fundamentals of Chemical Relaxation*, Verlag Chemie, Weinheim, New York, 1977.
5. J. M. Pechenik, *A Short Guide to Writing About Biology*, 9th Edition, Pearson.
6. Shah, M. A. and Ahmad, T., *Nanoscience and Nanotechnology*, I.K. International Publishing House Pvt. Ltd., 2021.
7. Egerton, R. F., *Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM*, 2nd Edition, Springer, 2016.
8. West, P. E., *Introduction to Atomic Force Microscopy*, Pacific Nanotechnology.
9. R. A. Robinson and R. H. Stokes, *Electrolyte Solutions*, 2nd Edition, Dover Publications.
10. D. N. Sathyanarayana, *Experimental Physical Chemistry*, Universities Press.
11. J. N. Gurtu and R. Kapoor, *Advanced Experimental Chemistry*, S. Chand & Company.
12. M. J. Rosen and J. T. Kunjappu, *Surfactants and Interfacial Phenomena*, 4th Edition, Wiley.
13. K. S. Birdi, *Handbook of Surface and Colloid Chemistry*, CRC Press.
14. B. E. Conway, J. O'M. Bockris and E. Yeager (Eds.), *Comprehensive Treatise of Electrochemistry*, Plenum Press.
15. P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, Oxford University Press.
16. D. P. Shoemaker, C. W. Garland and J. W. Nibler, *Experiments in Physical Chemistry*, McGraw–Hill.

MCH-3PL: Physical Chemistry Lab–III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3PL	8	200 (UE=100, IA=100)	Practical

1. **Spectroscopic Calculations**
   - (a) Verification of Beer–Lambert law.
   - (b) Determination of λ_{max}.
   - (c) Determination of concentration using UV–Visible spectroscopy.
   - (d) Determination of pK_a spectrophotometrically.
   - (e) Study of charge-transfer complexes.
2. **Electrochemistry**
   - (a) EMF measurements.
   - (b) Concentration cells.
   - (c) Verification of Nernst equation.
   - (d) Determination of transport number.
   - (e) Determination of ionic mobility.
3. **Thermochemistry**
   - (a) Zero-point energy.
   - (b) Enthalpy, entropy and Gibbs free energy.
   - (c) Reaction energy calculations.
   - (d) Solvent effects using continuum models.
   - (e) Heat of neutralization.
   - (f) Distribution law.
   - (g) Partition coefficient.
   - (h) Phase equilibrium.
   - (i) Cryoscopy/Ebullioscopy.
4. **Surface and Colloid Chemistry**
   - (a) Surface tension by stalagmometer.
   - (b) Critical micelle concentration.
   - (c) Adsorption isotherms.
   - (d) Viscosity measurements.
   - (e) Molecular weight determination by viscosity.
5. **Thermodynamics**
   - (a) Heat of neutralization.
   - (b) Distribution law.
   - (c) Partition coefficient.
   - (d) Phase equilibrium.
   - (e) Cryoscopy/Ebullioscopy.

6. **Instrumental Data Analysis**
   (a) Regression analysis.
   (b) Error propagation.
   (c) Scientific graph preparation using Origin or equivalent software.
7. **Scientific Presentation**
   (a) Preparation of scientific reports.
   (b) Data visualization.
   (c) Preparation of publication-quality figures.

MCH-3M1: Polymer Chemistry and Macromolecular Architecture

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3M1	3	100 (UE=60, IA=40)	Material Special (DSE)

Objective

To impart a fundamental understanding of polymerization mechanisms, polymer technology, and the structure, properties, and applications of natural, synthetic, and biodegradable polymers.

Unit I: Polymerization

Addition (chain) polymerization; free-radical addition polymerization; ionic polymerization; cationic polymerization; anionic polymerization; coordination polymerization; condensation (step) polymerization; polycondensation polymerization; polyaddition polymerization; ring-opening polymerization; copolymerization; free-radical copolymerization; monomer reactivity ratios; reactivity ratios and copolymerization behaviour; ionic copolymerization; group transfer polymerization; metathetical polymerization; electrochemical polymerization; Ziegler–Natta polymerization.

Unit II: Polymer Technology

Additives for plastics: fillers and reinforcements; plasticizers; antioxidants; heat stabilizers; ultraviolet stabilizers; flame retardants; colorants; chemical blowing agents; lubricants; microorganism inhibitors; curing agents; crosslinking agents. Properties and applications of thermoplastics and thermosetting polymers. Polymeric coatings.

Unit III: Biopolymers

Structure, functions and properties of naturally occurring polymers such as proteins, polysaccharides and DNA. Polymer chemistry of biological processes. Synthetic biopolymers, their fabrication and applications. Bioplastics and types of bioplastics. Natural biodegradable polymers, synthetic biodegradable polymers and modified naturally biodegradable polymers.

Essential Reading

1. Young, R. J., *Introduction to Polymers*, CRC Press.
2. Sperling, L. H., *Introduction to Physical Polymer Science*, 4th Edition, John Wiley & Sons.
3. Carraher, C. E., Jr., *Polymer Chemistry*, CRC Press.
4. Doi, M., *Introduction to Polymer Physics*, Oxford University Press.
5. Hiemenz, P. C. and Lodge, T. P., *Polymer Chemistry*, 2nd Edition, CRC Press.
6. Nadda, A. K., Sharma, S. and Bhat, R., *Biopolymers: Recent Updates, Challenges and Opportunities*, CRC Press.

MCH-3M2: Nanomaterials: Synthesis, Properties and Applications

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3M1	3	100 (UE=60, IA=40)	Material Special (DSE)

Objective

To provide a fundamental understanding of nanomaterials, their synthesis, characterization, green synthesis approaches, and emerging applications in materials science, energy, environment, and biotechnology.

Unit I: Introduction to Nanomaterials

Definition, scope, and classification of nanomaterials based on size, dimensionality, composition, origin, morphology, and size-dependent properties. Fundamental properties of nanomaterials with emphasis on surface area, shape, and surface energy. Optical, magnetic, mechanical, and electrical properties of nanomaterials and their correlation with reduced dimensionality, including quantum confinement effects and their influence on electronic structure and physical behaviour. Classification and detailed discussion of nanostructured materials with special reference to carbon-based nanomaterials such as carbon black, graphite, graphene, graphene oxide, and carbon nanotubes, along with fumed silica, quantum dots, metal nanoparticles, and other emerging nanostructures.

Unit II: Synthesis of Nanomaterials

Overview of top-down and bottom-up approaches for the synthesis of nanomaterials. Top-down methods including mechanical milling, lithographic techniques, and laser ablation, with emphasis on their principles, advantages, and limitations. Bottom-up approaches including sol–gel process, chemical vapour deposition (CVD), hydrothermal and solvothermal methods, and co-precipitation techniques, highlighting reaction parameters, growth mechanisms, and control over particle size and morphology. Introduction to greener and sustainable approaches for nanoparticle synthesis using environmentally benign reagents, energy-efficient processes, and biological or plant-mediated synthetic routes.

Unit III: Applications of Nanomaterials

Introduction to two-dimensional (2D) materials with emphasis on graphene, MXenes, and transition-metal dichalcogenides (TMDs), including their structures, properties, synthesis, and unique electronic and surface characteristics. Fundamentals of metal–organic frameworks (MOFs) and organic–inorganic hybrid materials, focusing on their design, structural diversity, tunability, and integration into functional systems. Applications of advanced functional materials in environmental remediation, particularly in photocatalysis and adsorption processes for pollutant removal and sustainable environmental management.

Essential Reading

1. Edelstein, A. S. and Cammarata, R. C., *Nanomaterials: Synthesis, Properties and Applications*, Institute of Physics (IOP) Publishing.
2. Ahmad, I., *Synthesis and Applications of Nanomaterials and Nanocomposites*, CRC Press.
3. He, J., *Nanostructured Materials: Synthesis, Properties and Applications*, Woodhead Publishing.
4. Vollath, D., *Nanomaterials: An Introduction to Synthesis, Properties and Applications*, 2nd Edition, Wiley–VCH.

5. Cao, G. and Wang, Y., *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, 2nd Edition, World Scientific.

6. Poole, C. P. Jr. and Owens, F. J., *Introduction to Nanotechnology*, Wiley–Interscience.

MCH-3M3: Hybrid Materials and Computational Frontiers

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3M1	3	100 (UE=60, IA=40)	Material Special (DSE)

Objective

This course integrates the theory and design of synergistic hybrid materials with practical computational chemistry techniques used to model, analyse, and predict their advanced electronic, optical, and reactive properties.

Unit I: Introduction to Hybrid Materials

Definition and historical development of hybrid materials; classification of Class I and Class II hybrid materials; inorganic precursors, organic polymers and functional additives; concept of synergistic property enhancement; synthesis strategies, structural features and applications of hybrid materials.

Unit II: Basics of Computational Chemistry

Introduction to computational chemistry and quantum chemistry; computational hardware, software and tools; Gaussian and GaussView; ORCA and Avogadro; input file preparation, job submission, output analysis and visualization. Vibrational spectral analysis using VEDA: theory and applications. Introduction to density functional theory (DFT), basis sets and computational workflows.

Unit III: Electronic Structure and Spectral Analysis

IR and Raman spectral plotting using computational tools; interpretation of IR and Raman spectra; UV–Visible spectral analysis: electronic transitions and spectral interpretation. Molecular Electrostatic Potential (MEP) analysis: visualization and interpretation. Electron Localization Function (ELF) analysis. Frontier molecular orbitals (HOMO–LUMO): energy gap, chemical reactivity and global reactivity descriptors. Nonlinear optical (NLO) properties: polarizability and hyperpolarizability.

Essential Reading

1. Levy, D. and Zayat, M. (Eds.), *Introduction to Hybrid Materials*, Wiley–VCH.
2. Cramer, C. J., *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition, John Wiley & Sons.
3. Foresman, J. B. and Frisch, A., *Exploring Chemistry with Electronic Structure Methods*, 3rd Edition, Gaussian Inc.
4. Sathyanarayana, D. N. (Ed.), *Vibrational Spectroscopy: Theory and Applications*, New Age International Publishers.
5. Papadopoulos, M. G., Sadlej, A. J. and Leszczynski, J. (Eds.), *Nonlinear Optical Properties of Matter: From Molecules to Condensed Phases*, Springer.
6. Jensen, F., *Introduction to Computational Chemistry*, 3rd Edition, John Wiley & Sons.

MCH-3M4: Materials for Energy Conversion and Storage

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3M1	3	100 (UE=60, IA=40)	Material Special (DSE)

Objective

To provide an advanced understanding of the design, synthesis, characterization, and applications of emerging nanomaterials for sustainable energy conversion, storage, and environmental applications.

Unit I: Advanced Carbon Nanostructures and Perovskite Materials

Carbon-based nanomaterials: graphene oxide (GO), reduced graphene oxide (rGO), carbon nanotubes (CNTs), and quantum dots (QDs); structure, properties and applications; composites of carbon-based nanostructured materials; functionalization of carbon-based nanomaterials.

Introduction and general background of perovskites; crystal structure and properties of perovskites; device architectures and processing; photovoltaic principles: working principles of solar cells and p–n junctions; charge generation, transport and recombination processes in perovskite semiconductors.

Unit II: MXene-Based Materials and Energy Applications

Introduction and fundamentals of MXenes; structure, properties and synthesis of MXenes; applications of MXenes in energy storage and energy conversion; MXene-based hybrid materials: fabrication, morphology and electrochemical energy storage performance.

Introduction and fundamentals of metal oxides and their composites; metal oxides for energy storage and conversion; introduction to metal–organic frameworks (MOFs); structure and properties of MOFs; metal oxide-integrated metal–organic frameworks; applications of MOFs in electrochemical energy storage and conversion.

Unit III: Advanced Nanomaterials for Sustainable Energy Systems

Hydrogen production through photocatalytic water splitting and photoelectrochemical water splitting; advanced nanomaterials for batteries, solar cells, fuel cells and hydrogen storage; nanomaterials as electrode materials for fuel cells; supercapacitors; photocatalytic and electrocatalytic materials for renewable energy technologies.

Essential Reading

1. Jun, H. K. and Low, F. W., *Materials for Energy Conversion and Storage*, CRC Press.
2. Cheong, K. Y., Fraga, G. I. and Amorim, M., *Emerging Materials for Energy Conversion and Storage*, Elsevier.
3. Sonkar, P. K., Ganesan, V. and Vellachamy, V., *Advancements in Nanomaterials for Energy Conversion and Storage*, Springer.
4. Naik, R., Nagaswarupa, H. P., Murthy, H. C. A. and Sillanpää, M., *Advanced Nanomaterials for Energy Storage Devices*, Elsevier.
5. Cao, G. and Wang, Y., *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, 2nd Edition, World Scientific.
6. Poole, C. P. Jr. and Owens, F. J., *Introduction to Nanotechnology*, Wiley–Interscience.

MCH-3M5: Research Methodology (Material Branch)

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3M5	4	100 (UE=60, IA=40)	Theory (Material (RM))

Objective

To provide a comprehensive understanding of the complete research workflow encompassing laboratory safety, advanced materials synthesis, computational characterization, rigorous data analysis, and effective scientific communication.

Unit I: Laboratory Safety and Precautions

General laboratory instructions and safety practices. Chemical hazards and hazard management; hazard identification; Safety Data Sheets (SDS) and Material Safety Data Sheets (MSDS); Globally Harmonized System (GHS) of classification and labelling of chemicals. Safe handling, storage and disposal of chemicals; waste management; laboratory equipment and operational safety; precautionary measures for the maintenance of laboratory equipment; safe handling of glassware; electrical safety; laboratory ventilation; emergency preparedness and response.

Unit II: Experimental Methods

Formulation of research problems; stages of the research process; preparation of research design. Synthesis of advanced materials; crystal structure determination; Hirshfeld surface analysis; density functional theory (DFT) calculations and prediction of nonlinear optical (NLO)-active compounds; time-dependent density functional theory (TD-DFT) analysis; frontier molecular orbital (HOMO–LUMO) energy gap; local and global reactivity descriptors; introduction to molecular docking and molecular dynamics (MD) simulations.

Unit III: Data Interpretation and Result Discussion

Data analysis: arithmetic mean, standard deviation, absolute and relative errors; linear regression; covariance and correlation coefficient; precision, accuracy and error analysis; variance and chi-square test; graphical representation and interpretation of experimental and computational data using scientific software.

Unit IV: Dissemination of Research Findings

Presentation of research findings; preparation of scientific reports and research publications; seminar presentation; patent writing; research paper writing; journal impact factor, CiteScore, h-index and i10-index; peer-review process; ethics in scientific publishing.

Essential Reading

1. Prathapan, K., *Research Methodology for Scientific Research*, Dreamtech Press, 2019.
2. Ridley, R., *Handbook of Good Laboratory Practices*, 2nd Edition, World Health Organization (WHO), 2009.
3. Kumari, R., *Computers and Their Applications to Chemistry*, 2nd Edition, Narosa Publishing House, 2007.
4. Atkinson, K., *Elementary Numerical Analysis*, 2nd Edition, John Wiley & Sons, 2003.
5. Harris, D. C., *Quantitative Chemical Analysis*, 10th Edition, W. H. Freeman.
6. Cramer, C. J., *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition, John Wiley & Sons.

MCH-3ML: Material Chemistry Lab–III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCH-3ML	8	200 (UE=100, IA=100)	Practical

Experiments

1. Methods of preparation of single crystals.
2. Determination of packing in crystals.
3. Analysis of materials by X-ray powder diffraction (XRD).
4. Green synthesis of pure and doped semiconductors.
5. Synthesis of n-type and p-type semiconductor materials.
6. Synthesis of cobalt ferrite ($CoFe_2O_4$) inverse spinel by chemical route.
7. Synthesis and measurement of the dielectric constant of barium titanate ($BaTiO_3$).

Reference Books

1. Laboratory manual prepared by the Teacher-in-Charge.

MCH-4I1: Advanced Inorganic Spectroscopy

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4I1	2	50 (UE=30, IA=20)	Inorganic Special (DSE)

Objective: Advances in inorganic spectroscopy

Unit I: Multi-nuclear Magnetic Resonance Spectroscopy

Nuclear spin quantum number (I). Types of nuclei based on the value of I. Measurement of chemical shifts and factors affecting chemical shift values. Application of chemical shifts, signal intensities and spin–spin splitting for structural determination of inorganic compounds carrying NMR-active nuclei such as ^{1}H, ^{11}B, ^{15}N, ^{19}F, ^{31}P, etc. Chemical exchange and other factors affecting line width.

Unit II: Molecular Spectroscopy in Inorganic Molecules

(a) Mössbauer Spectroscopy

Doppler shift and recoil energy. Isomer shift and its interpretation. Quadrupole interactions. Effect of magnetic field on Mössbauer spectra. Applications to metal complexes, metal carbonyls, Fe–S clusters and tin compounds. Partial quadrupole splitting and geometry of complexes.

(b) Mass Spectrometry

Experimental arrangements and presentation of spectra. Molecular ions, appearance and ionization potential. Fragmentation, ion reactions and their interpretation. Fingerprint applications and interpretation of mass spectra. Effect of isotopes on the appearance of mass spectra. Molecular weight determination. Evaluation of heats of sublimation and species in the vapour over high melting solids, and thermodynamic data.

Essential Reading

1. Drago, R. S., *Physical Methods for Chemists*, 2nd Edition, East West Press Pvt. Ltd., 2016.

2. *Mass Spectrometry: Principles and Applications*, 3rd Edition, Wiley.

MCH-4I2: Stereochemistry and Metal Ion Catalysis

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4I2	2	50 (UE=30, IA=20)	Inorganic Special (DSE)

Objective: Concepts in stereochemistry and metal ion catalysis

Unit I: Stereochemical Changes in Octahedral Complexes

Outer-sphere orientations. Reactions of geometrical and optical isomers. S_N1 dissociation and S_N2 displacement mechanisms. Stereochemistry of acid- and base-catalysed hydrolysis of Co(III) complexes. Optical inversion reactions of selected Co(III) complexes.

Unit II: Metal Ion Catalysis

Metal ion catalysis in acid–base reactions. Acid catalysis of hydrolysis, aldol condensation, carboxylation and decarboxylation reactions. Metal ion catalysis in redox reactions. Autoxidation of organic substances.

Essential Reading

1. Basolo, F. and Pearson, R. G., *Mechanisms of Inorganic Reactions*, Wiley.
2. Edwards, J. O., *Inorganic Reaction Mechanisms*, Wiley.
3. Langford, C. H. and Gray, H. B., *Ligand Substitution Processes*, W. A. Benjamin.

MCH-4I3: Advanced Organometallic Chemistry–II

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4I3	2	50 (UE=30, IA=20)	Inorganic Special (DSE)

Objective: Advanced organometallic chemistry

Unit I: Fluxionality, Dynamic Equilibria and Distinctive Organometallic Reactions

Stereochemical non-rigidity in organometallic complexes. Scrambling of carbonyl groups in metal carbonyl complexes. Fluxionality and dynamic equilibria in olefinic, π-allyl and cyclopentadienyl complexes.
Oxidative addition reactions in d^{10}, d^8 and d^7 complexes. Intramolecular oxidative addition reactions. C–H activation, cyclometallation and ortho-metallation. Oxidative coupling reactions. Reductive elimination reactions in mono- and binuclear systems. α- and β-elimination reactions. β-Hydrogen elimination and β-hydrogen transfer reactions. Insertion reactions: insertion of carbonyls and alkenes; migratory insertion reactions.

Unit II: Transition Metal–Carbon Multiple Bonds and Catalytic Applications of Organometallic Complexes

Transition metal carbene complexes: Fischer carbenes and Schrock carbenes, their requisites and properties. Tebbe's reagent. Intermediate carbenes between Fischer and Schrock types. Grubbs' catalysts (first and second generation) and their applications.
Transition metal carbyne complexes: preparation, properties and structures.
Catalytic applications of organometallic complexes: alkene hydrogenation and Wilkinson catalyst; synthesis gas (H_2/CO) formation; Monsanto acetic acid process; hydroformylation reactions; Wacker oxidation process and isomerisation; polymerisation reactions and Ziegler–Natta catalysis.

Essential Reading

1. Pearson, A. J., *Metallo-organic Chemistry*, John Wiley & Sons Inc., 1985.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edition, Harper Collins, 2005.
3. Tsutsui, M., Levy, M. N., Nakamura, A., Ichikawa, M. and Mori, K., *Introduction to Metal π-Complex Chemistry*, Plenum Press, New York, 1970.
4. Mehrotra, R. C. and Singh, A., *Organometallic Chemistry*, Wiley Eastern Ltd., 2000.
5. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., *Advanced Inorganic Chemistry*, 6th Edition, John Wiley & Sons Inc., 1999.
6. *Basic Organometallic Chemistry: Concepts, Syntheses and Applications.*

MCH-4I4: Comprehensive Bioinorganic Chemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4I4	2	50 (UE=30, IA=20)	Inorganic Special (DSE)

Objective: Concepts in bioinorganic mechanisms

Unit I: Transport and Function of Alkali and Alkaline Earth Metals

Functions of alkali and alkaline earth metal ions in biological systems. Role of alkali and alkaline earth metals in neuro-sensation. Ion channels and ion pumps. Magnesium-catalysed phosphate transfer reactions. Ubiquitous regulatory role of calcium ions in biological processes.

Unit II: Applications of Metal Ions in Biology

Medicinal and therapeutic applications of metal ions. Metal deficiency and related diseases. Toxic effects of metals. Metals used for diagnosis and chemotherapy. Gold compounds as anti-rheumatic agents.
Nitrogen cycle: biological nitrogen fixation. Role of metalloenzymes in the biological nitrogen cycle. Molybdenum nitrogenase and other nitrogenase model systems.

Essential Reading

1. Lippard, S. J. and Berg, J. M., *Principles of Bioinorganic Chemistry*, University Science Books.
2. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S., *Bioinorganic Chemistry*, University Science Books.
3. Eichhorn, G. L. (Ed.), *Inorganic Biochemistry*, Vols. I and II, Elsevier.

MCH-4O1: Medicinal Chemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4O1	2	50 (UE=30, IA=20)	Organic Special (DSE)

Unit I: Drug Design and Development

Concept of lead compounds, lead modification, prodrugs and soft drugs; structure–activity relationship (SAR); factors affecting bioactivity; electronic effects (resonance and inductive effects); receptor site theory; isosterism and bioisosterism; spatial considerations; occupancy theory, rate theory and induced-fit theory; concepts of drug receptors. Free–Wilson analysis, Hansch analysis and the relationship between Free–Wilson and Hansch analyses. Synthesis of selected therapeutic agents: tolmetin, chloramphenicol, tolazamide, diclofenac, oxaprozin, sulconazole, warfarin, diazepam and acyclovir. LD_{50} and ED_{50}.

Unit II: Mechanism of Drug Action and Chemotherapeutics

Mechanism of enzyme stimulation and inhibition; types of enzyme inhibition; antimetabolites (sulphonamides) and their classification; synthesis of penicillin G, ampicillin, tetracycline, ciprofloxacin and norfloxacin. Drug metabolism: Phase I (oxidation, reduction and hydrolysis) and Phase II (conjugation) reactions. Cardiovascular drugs: synthesis and mechanism of action of amyl nitrite, isosorbide dinitrate, diltiazem and pindolol. Drug chemotherapeutics and pharmacodynamic agents.

Books Suggested

1. A. Gringauz, *Introduction to Medicinal Chemistry*, Wiley–VCH.
2. R. B. Silverman and M. W. Holladay, *The Organic Chemistry of Drug Design and Drug Action*, 3rd Edition, Academic Press.
3. D. Lednicer, *Strategies for Organic Drug Synthesis and Design*, John Wiley & Sons.
4. S. N. Pandeya and J. R. Dimmock, *A Textbook of Medicinal Chemistry*, Vols. I & II, S. G. Publishers.
5. Ashutosh Kar, *Medicinal Chemistry*, 5th Edition, New Age International Publishers.
6. L. L. Brunton, R. Hilal-Dandan and B. C. Knollmann (Eds.), *Goodman & Gilman's The Pharmacological Basis of Therapeutics*, 14th Edition, McGraw–Hill.
7. M. E. Wolff (Ed.), *Burger's Medicinal Chemistry and Drug Discovery*, Vols. I–V, John Wiley & Sons.

MCH-4O2: Advanced Methods in Organic Synthesis

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4O2	2	50 (UE=30, IA=20)	Organic Special (DSE)

Unit I: Radical Chemistry

Introduction to radical chemistry; generation of free radicals; addition to π-bonds; fragmentation; atom abstraction; radical–radical combination; disproportionation; single-electron transfer (SET); nucleophilic radical addition and radical substitution reactions. Named reactions involving radicals: Sandmeyer reaction, Hunsdiecker reaction, Kolbe electrolysis, Minisci reaction, Kagan–Molander coupling, Dowd–Beckwith ring expansion, Keck radical allylation, Wohl–Ziegler bromination, Markó–Lam deoxygenation, Ueno–Stork cyclization and Zard radical aminomethylation.

Unit II: Carbenoids and *N*-Heterocyclic Carbenes (NHCs)

Introduction to carbenoids and carbenes; Fischer and Schrock carbenes and their synthetic applications; Dötz benzannulation and related reactions. Structure, electronic properties and reactivity of *N*-heterocyclic carbenes (NHCs); synthesis of NHCs via imidazolium salts and transition-metal NHC complexes; steric and electronic properties, basicity and decomposition pathways of NHCs. Applications of NHCs in organocatalysis and transition-metal catalysis. Carbene-mediated reactions involving C–H, N–H and O–H bond functionalization. Olefin metathesis: ring-closing metathesis (RCM), ring-opening metathesis (ROM), ring-opening metathesis polymerization (ROMP), enyne metathesis (EYM), ring-closing enyne metathesis (RCEYM), cross metathesis (CM) and tandem metathesis.

Books Suggested

1. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edition, Cambridge University Press, 2004.
2. R. Brückner, *Advanced Organic Chemistry: Reaction Mechanisms*, Elsevier, 2002.
3. J. Clayden, N. Greeves and S. Warren, *Organic Chemistry*, 2nd Edition, Oxford University Press, 2012.
4. S. Díez-González (Ed.), *N-Heterocyclic Carbenes: From Laboratory Curiosities to Efficient Synthetic Tools*, 2nd Edition, Royal Society of Chemistry, 2016.
5. R. H. Grubbs and A. G. Wenzel (Eds.), *Handbook of Metathesis*, 2nd Edition, Wiley–VCH, 2015.

MCH-4O3: Natural Products and Structural Elucidation

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4O3	2	50 (UE=30, IA=20)	Organic Special (DSE)

Unit I: Terpenoids, Alkaloids and Steroids

Introduction, occurrence, classification and nomenclature of terpenoids; isoprene rule and biogenesis of terpenoids; Diels' hydrocarbon. General methods for structure elucidation of representative terpenoids: citral, geraniol, menthol, zingiberene, camphor and longifolene. Alkaloids: occurrence, classification, general methods of structure determination and synthesis of ephedrine, nicotine, atropine, morphine and quinine. Steroids: nomenclature, stereochemistry and general methods of structure determination; synthesis and biological importance of estrone, androsterone and progesterone. Introduction to carotenoids: classification, structure and biological significance.

Unit II: Prostaglandins and Flavonoids

Introduction, occurrence, classification and nomenclature of prostaglandins and flavonoids. General methods of structure determination and synthesis of representative flavonoids including apigenin, luteolin, quercetin, myricetin, daidzein, flavones, flavonols and quinones. Stereochemistry, biosynthesis and biological significance of prostaglandins, thromboxanes and leukotrienes.

Books Recommended

1. I. L. Finar, *Organic Chemistry*, Vol. II, 6th Edition, Pearson Education.
2. J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harborne, *Natural Products: Their Chemistry and Biological Significance*, Longman Scientific & Technical.
3. B. A. Bohm, *Introduction to Flavonoids*, Harwood Academic Publishers.
4. O. P. Agarwal, *Chemistry of Organic Natural Products*, Vols. I & II, Goel Publishing House.
5. S. Coffey (Ed.), *Rodd's Chemistry of Carbon Compounds*, Elsevier.
6. M. Nogradi, *Stereoselective Synthesis: A Practical Approach*, VCH Publishers.
7. A. R. Battersby and T. W. Goodwin (Eds.), *Biosynthesis of Natural Products*, Wiley.
8. M. P. Gupta and A. Marston (Eds.), *Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas*, Harwood Academic Publishers.
9. Dewick, P. M., *Medicinal Natural Products: A Biosynthetic Approach*, 3rd Edition, John Wiley & Sons.

MCH-4O4: Organic spectroscopy

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4O4	2	50 (UE=30, IA=20)	Organic Special (DSE)

Unit I: Applications of ^1H and ^{13}C NMR Spectroscopy

First-order and non-first-order spectra; spin–spin coupling involving two, three, four and five nuclei (first-order treatment); coupling constants (J); classification of spin systems (AB, AX, AX_2, ABX, AMX, ABC and AB_2); resolution and multiplicity in ^{13}C NMR spectra; proton-decoupled and off-resonance decoupled ^{13}C NMR spectra; selective decoupling; broad-band decoupling; noise decoupling; heteronuclear coupling involving ^2H, ^{19}F and ^{31}P; structural applications of ^1H and ^{13}C NMR spectroscopy.

Unit II: Two-Dimensional NMR Spectroscopy

Introduction to two-dimensional (2D) NMR spectroscopy; APT, INEPT and DEPT experiments. Homonuclear correlation spectroscopy: COSY (^1H–^1H), TOCSY and NOESY. Heteronuclear correlation spectroscopy: HSQC, HMQC and HMBC. Homo- and heteronuclear 2D resolved spectroscopy. INADEQUATE experiment. Applications of multidimensional NMR spectroscopy in structural elucidation of organic molecules and biomolecules.

Books Suggested

1. W. Kemp, *Organic Spectroscopy*, 3rd Edition, Palgrave Macmillan.
2. R. M. Silverstein, F. X. Webster, D. J. Kiemle and D. L. Bryce, *Spectrometric Identification of Organic Compounds*, 9th Edition, John Wiley & Sons.
3. M. L. Martin, J. J. Delpuech and G. J. Martin, *Practical NMR Spectroscopy*, Heyden & Son Ltd.
4. R. J. Abraham, J. Fisher and P. Loftus, *Introduction to NMR Spectroscopy*, John Wiley & Sons.
5. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
6. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 8th Edition, McGraw–Hill Education.
7. H. Friebolin, *Basic One- and Two-Dimensional NMR Spectroscopy*, 5th Edition, Wiley–VCH.
8. E. Breitmaier, *Structure Elucidation by NMR in Organic Chemistry: A Practical Guide*, 3rd Edition, Wiley.

MCH-4P1: Non-Equilibrium Statistical Mechanics and Biophysical Systems

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4P1	2	50 (UE=30, IA=20)	Physical Special (DSE)

Unit I: Non-Equilibrium Statistical Mechanics and Stochastic Dynamics 25L

Limitations of equilibrium statistical mechanics and motivation for non-equilibrium descriptions. Random walks and Brownian motion. Stochastic forces and noise: Gaussian and white noise, noise correlations, and Markovian processes.
Langevin equation for a free particle and for a particle in an external potential. Velocity autocorrelation function. Mean-square displacement and diffusion processes. Overdamped limit and the Smoluchowski equation. Einstein relation and equipartition theorem.
Derivation of the Fokker–Planck equation from Langevin dynamics. Time-dependent and stationary probability distributions. Relaxation to equilibrium and the principle of detailed balance.
Linear response theory and the fluctuation–dissipation theorem. Non-equilibrium steady states: probability currents and entropy production. Master equations for two-state and multi-state systems.
Introductory stochastic thermodynamics: work, heat, and entropy along stochastic trajectories. Qualitative introduction to fluctuation theorems.
Numericals: mean-square displacement, diffusion coefficient, steady-state probabilities, relaxation times, correlation and response functions.

Unit II: Biophysical Chemistry and Molecular Simulations 25L

Fundamental interactions governing biomolecular structure and stability: hydrogen bonding, electrostatic and van der Waals interactions, hydrophobic effects, and stereoelectronic contributions. Role of water in biological systems: polarity, dielectric constant, hydrogen bonding network, hydration forces, and solvent-mediated interactions.
Thermodynamic principles of biomolecular stability and conformational equilibria: enthalpy, entropy, Gibbs free energy, and enthalpy–entropy compensation.
Amino acids and peptide bond formation. Hierarchical organization of protein structure: primary, secondary (α-helix and β-sheet), tertiary, and quaternary structures. Polypeptide chain geometry: bond lengths, bond angles, torsion angles ϕ, ψ, and ω. Ramachandran plot: allowed and disallowed regions and its role in protein structure validation.
Nucleic acids: nucleosides and nucleotides; structure of DNA and RNA; base pairing, base stacking, and structural polymorphism (A-, B-, and Z-DNA).
Statistical mechanics of macromolecular chains: random walk and freely jointed chain models. End-to-end distance, radius of gyration, Gaussian chain model, and entropic elasticity. Ideal and real polymer chains; excluded volume effects (qualitative). Flory mean-field theory and Flory–Huggins theory of polymer solutions.
Conformational transitions: helix–coil transition and qualitative aspects of protein folding. Introductory polymer dynamics: Rouse model (conceptual).
Molecular mechanics and molecular dynamics simulations of biomolecules and polymers: potential energy surfaces, bonded and non-bonded interactions, force fields, energy minimization, and basic time-integration algorithms (Verlet and velocity-Verlet: qualitative).
Numericals: radius of gyration, mean-square end-to-end distance, force–extension relations, scaling exponents.

Essential Reading

1. van Kampen, N. G., *Stochastic Processes in Physics and Chemistry*, Elsevier.

2. Gardiner, C. W., *Handbook of Stochastic Methods*, Springer.
3. Risken, H., *The Fokker–Planck Equation*, Springer.
4. Kubo, R., Toda, M., and Hashitsume, N., *Statistical Physics II*, Springer.
5. Seifert, U., "Stochastic Thermodynamics, Fluctuation Theorems and Molecular Machines", *Reports on Progress in Physics.*
6. Cantor, C. R. and Schimmel, P. R., *Biophysical Chemistry*, Vols. I–III, W. H. Freeman.
7. Volkenstein, M. V., *Molecular Biophysics*, Academic Press.
8. Creighton, T. E., *Proteins: Structures and Molecular Properties*, W. H. Freeman.
9. Frenkel, D. and Smit, B., *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press.
10. Allen, M. P. and Tildesley, D. J., *Computer Simulation of Liquids*, Oxford University Press.

MCH-4P2: Advanced Molecular Spectroscopy

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4P2	2	50 (UE=30, IA=20)	Physical Special (DSE)

Unit I: Fundamentals & Quantum Background of Spectroscopy 10L

Time-dependent perturbation theory; Einstein coefficients; Lambert–Beer law; integrated absorption coefficients; oscillator strength; transition dipole moments; general selection rules based on symmetry principles. Qualitative interpretation of UV–Visible spectra of polyatomic organic molecules (e.g., ethene, formaldehyde, *cis*- and *trans*-butadiene) using symmetry principles.

Unit II: Vibrational and Magnetic Resonance Spectroscopy 10L

Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules such as BF_3 and NH_3. Vibrational analysis of square-planar, trigonal bipyramidal, framework and cage molecules. Jahn–Teller distortions.
NMR Spectroscopy: Mechanism of spin–spin and spin–lattice relaxation processes; quantitative treatment of relaxation phenomena; quantum mechanical treatment of the AB spin system; selection rules and relative intensities of spectral lines.
ESR Spectroscopy: Applications of ESR spectroscopy in structure determination; interpretation of ESR spectra of simple organic radicals such as benzene radical anion, naphthalene radical anion, toluene radical cation and *o*-, *m*- and *p*-xylene radical ions using Hückel Molecular Orbital (HMO) theory; study of unstable paramagnetic species; kinetic studies of electron-transfer reactions.

Suggested Reading

1. D. C. Harris and M. D. Bertolucci, *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover Publications, New York, 1990.
2. D. M. Bishop, *Group Theory and Chemistry*, Clarendon Press, Oxford, 1973.
3. A. Carrington and A. D. McLachlan, *Introduction to Magnetic Resonance*, Chapman & Hall, New York, 1983.
4. J. E. Wertz and J. R. Bolton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman & Hall, New York, 1986.
5. R. Chang, *Basic Principles of Spectroscopy*, McGraw–Hill, New York, 1971.

MCH-4P3: Advanced Electrochemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4P3	2	50 (UE=30, IA=20)	Physical Special (DSE)

Unit I: Electrolyte Solutions and Electrode Kinetics 15L

Structure of water and hydrogen-bonded network. Effect of ions on the structure of water. Electrochemical potential and activities of ions. Limiting laws for electrolyte solutions. Derivation of the Debye–Hückel–Onsager equation.
Charge transfer processes at electrodes: charge transfer under zero electric field and under the influence of an applied electric field. Two-way electron transfer reactions. Equilibrium exchange current density. Interface under non-equilibrium conditions.
Derivation of the Butler–Volmer equation. Tafel equation and Tafel plots. Electrode kinetics involving multistep reactions.

Unit II: Transport Phenomena and Electrical Double Layer 15L

Diffusion coefficients and ionic mobility. Fick's first law of steady-state diffusion and Fick's second law of non-steady-state diffusion. Einstein relation between diffusion coefficient and absolute mobility of ions. Stokes–Einstein equation. Nernst–Einstein equation.
Nernst–Planck flux equation and ionic transport in electrolyte solutions. Electrical double layer at the electrode–electrolyte interface. Thermodynamics of electrified interfaces.
Derivation of the electrocapillary equation. Determination of charge density on electrodes. Electrical capacitance of the electrode–electrolyte interface.

Essential Reading

1. Bockris, J. O'M. and Reddy, A. K. N., *Modern Electrochemistry*, Vol. 1: Ionics, 2nd Ed., Plenum Press, New York, 1998.

2. Bockris, J. O'M., Reddy, A. K. N., and Gamboa-Aldeco, M., *Modern Electrochemistry*, Vol. 2A: Fundamentals of Electrodics, 2nd Ed., Plenum Press, New York, 2000.

3. Bard, A. J. and Faulkner, L. R., *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley & Sons, New York, 2002.

MCH-4P4: Nanochemistry

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4P4	2	50 (UE=30, IA=20)	Physical Special (DSE)

Unit I: Fundamentals, Properties and Applications of Nanomaterials 15L

Perspective of length scales and emergence of nanoscience. Nanomaterials and chemistry of advanced materials and nanostructures. Solid materials and their strength at the nanoscale; surface effects and size-dependent properties.
Carbon nanostructures: graphene, fullerenes, and carbon nanotubes (SWCNT and MWCNT). Surface plasmon resonance and quantum size effects.
Applications of nanomaterials based on noble metals (gold and silver), dielectric and magnetic oxides. Applications in health and medicine, environment and water purification, automobiles, sensors, batteries, computers, communication, food, paints, textiles, and ceramic industries.
Functional applications: nanocatalysis, photocatalysis, electrocatalysis, photoelectrocatalysis, water splitting, and green and renewable energy.

Unit II: Synthesis and Characterization of Nanomaterials 15L

Overview of synthesis routes: solvothermal and hydrothermal methods, reverse micellar and microemulsion techniques, sol–gel process, polymeric citrate precursor method, co-precipitation, and sonochemical methods. Theory, experimental conditions, and kinetics of solid-state and molten-salt routes.
Structural characterization using X-ray diffraction: Laue and powder methods. Particle size determination using X-ray line broadening and Scherrer's formula.
Theory, instrumentation, and applications of SEM, TEM, AFM, and STM. Principles and methodology of dynamic light scattering (DLS) and Brunauer–Emmett–Teller (BET) surface area analysis.

Essential Reading

1. Shah, M. A. and Ahmad, T., *Principles of Nanoscience and Nanotechnology*, Narosa Publishing House, New Delhi, 2010.
2. Viswanathan, B., *Nanomaterials*, Narosa Publishing House, New Delhi, 2009.
3. Pradeep, T., *Nano: The Essentials*, Tata McGraw–Hill, New Delhi, 2009.
4. Rao, C. N. R., Müller, A., and Cheetham, A. K. (Eds.), *Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Wiley–VCH, Weinheim, 2004.
5. Liz–Marzán, L. M. and Kamat, P. V., *Nanoscale Materials*, Kluwer Academic Publishers, Boston, 2003.

MCH-4M1: Functional Materials (Optical, Electronic and Magnetic)

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4M1	2	50 (UE=30, IA=20)	Material Special (DSE)

Objective

This course introduces the quantum mechanical principles governing the electronic, magnetic and optical properties of solids, with emphasis on their applications in modern electronic, photonic and energy devices.

Unit I: Electronic Properties of Solids

Electronic structure of solids; free electron theory and its limitations; nearly-free electron model; band theory of solids; reciprocal lattice, Brillouin zones and k-space; energy bands in metals, semiconductors and insulators; intrinsic and extrinsic semiconductors; carrier concentration and mobility; doped semiconductors; p–n junctions and semiconductor devices (qualitative treatment); Hall effect; superconductivity, Meissner effect and critical parameters; introduction to Bardeen–Cooper–Schrieffer (BCS) theory.

Unit II: Magnetic and Optical Properties of Solids

Magnetic Properties: Magnetic susceptibility; Langevin theory of diamagnetism and paramagnetism; Curie and Curie–Weiss laws; origin of magnetic moments; exchange interaction; ferromagnetism, antiferromagnetism and ferrimagnetism; magnetic domains; hysteresis; soft and hard magnetic materials; magnetic materials for data storage.
Optical Properties: Interaction of electromagnetic radiation with solids; optical absorption and emission; colour centres; excitons; photoluminescence and electroluminescence; light-emitting diodes (LEDs), laser diodes, GaAs lasers, photovoltaic (solar) cells, optical fibres, photonic crystals, metamaterials and quantum wells; refractive index and optical dispersion.

Books Suggested

1. N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Brooks/Cole.
2. C. Kittel, *Introduction to Solid State Physics*, 8th Edition, John Wiley & Sons.
3. M. Fox, *Optical Properties of Solids*, 2nd Edition, Oxford University Press.
4. D. A. Neamen, *Semiconductor Physics and Devices: Basic Principles*, 4th Edition, McGraw–Hill.
5. K. H. J. Buschow and F. R. de Boer, *Physics of Magnetism and Magnetic Materials*, Springer.
6. J. I. Pankove, *Optical Processes in Semiconductors*, Dover Publications.
7. S. O. Kasap, *Principles of Electronic Materials and Devices*, 4th Edition, McGraw–Hill.

MCH-4M2: Advanced Characterization Techniques

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4M2	2	50 (UE=30, IA=20)	Material Special (DSE)

Objective

This course provides a comprehensive understanding of the principles, instrumentation, working methodologies and applications of modern microscopy, spectroscopy, diffraction and scattering techniques for the structural, morphological, chemical and electronic characterization of materials from the atomic to the macroscopic scale.

Unit I: Microscopy and Imaging Techniques

Principles, instrumentation and applications of optical microscopy; fluorescence microscopy; confocal laser scanning microscopy (CLSM); scanning electron microscopy (SEM); field-emission scanning electron microscopy (FESEM); transmission electron microscopy (TEM); high-resolution transmission electron microscopy (HRTEM); cryogenic transmission electron microscopy (Cryo-TEM); scanning transmission electron microscopy (STEM); atomic force microscopy (AFM); scanning tunneling microscopy (STM); helium ion microscopy (HIM); energy dispersive X-ray spectroscopy (EDS/EDX) attached to electron microscopes; elemental mapping and electron diffraction.

Unit II: Spectroscopy, Diffraction and Scattering Techniques

X-ray diffraction (XRD): principles, instrumentation and phase identification; crystallite size and lattice strain analysis; X-ray photoelectron spectroscopy (XPS); Fourier-transform infrared spectroscopy (FTIR); Raman and tip-enhanced Raman spectroscopy (TERS); ultraviolet–visible diffuse reflectance spectroscopy (UV–Vis DRS); photoluminescence spectroscopy (PL); dynamic light scattering (DLS); small-angle X-ray scattering (SAXS); X-ray absorption spectroscopy (XAS), including XANES and EXAFS (introductory treatment); applications of multimodal characterization in nanomaterials, polymers, catalysts and energy materials.

Essential Reading

1. Douglas B. Murphy and Michael W. Davidson, *Fundamentals of Light Microscopy and Electronic Imaging*, 2nd Edition, Wiley.
2. Peter W. Hawkes and John C. H. Spence (Eds.), *Springer Handbook of Microscopy*, Springer.
3. Yoshio Waseda, Eiichiro Matsubara and Kozo Shinoda, *X-Ray Diffraction Crystallography: Introduction, Examples and Solved Problems*, Springer.
4. Manuel Nieto-Vesperinas, *Scattering and Diffraction in Physical Optics*, 2nd Edition, World Scientific.
5. Harekrushna Sahoo, *Optical Spectroscopic and Microscopic Techniques*, Springer.
6. Brent Fultz and James Howe, *Transmission Electron Microscopy and Diffractometry of Materials*, 4th Edition, Springer.
7. C. Barry Carter and David B. Williams, *Transmission Electron Microscopy: A Textbook for Materials Science*, 2nd Edition, Springer.
8. John F. Watts and John Wolstenholme, *An Introduction to Surface Analysis by XPS and AES*, Wiley.

MCH-4M3: Basics in Crystallography

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4M3	2	50 (UE=30, IA=20)	Material Special (DSE)

Objective

To provide a comprehensive understanding of crystal symmetry, crystal structures, space-group symmetry, and diffraction principles for the structural characterization of crystalline materials.

Unit I: Crystal Lattices and Unit Cells

Crystal lattices and unit cells; crystal systems and Bravais lattices; lattice parameters; crystal symmetry and symmetry elements; Hermann–Mauguin notation for symmetry elements; point, line and plane symmetry; screw axes and glide planes; lattice planes and directions; Miller and Weiss indices; interplanar spacing; crystal forms and zones; hexagonal crystal system; indexing of crystal planes in hexagonal systems; reciprocal lattice (introductory treatment).

Unit II: Point Groups and Space Groups in Crystallography

Point groups in crystallography; Hermann–Mauguin notation of crystallographic point groups; centrosymmetric and non-centrosymmetric point groups; crystal classes; stereographic projection (introductory treatment); space groups and translational symmetry; generation of space groups from symmetry operations; structural interpretation of representative space groups including P1, P$\bar{1}$, P2, P2_1, C2, C2/m, P2_1/c, P$2_1 2_1 2_1$, I4_1, P6_3/mmc and Fm$\bar{3}$m. Applications of crystallographic symmetry in crystal structure determination.

Books Suggested

1. Gale Rhodes, *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models*, 3rd Edition, Academic Press.
2. Donald E. Sands, *Introduction to Crystallography*, Dover Publications.
3. C. Giacovazzo (Ed.), *Fundamentals of Crystallography*, 3rd Edition, Oxford University Press.
4. Theo Hahn (Ed.), *International Tables for Crystallography, Volume A: Space-Group Symmetry*, International Union of Crystallography (IUCr).
5. Marc De Graef and Michael E. McHenry, *Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry*, 3rd Edition, Cambridge University Press.
6. L. Monoceros Boas, *Crystal Structures: Patterns and Symmetry*, Mineralogical Society of America.
7. B. D. Cullity and S. R. Stock, *Elements of X-Ray Diffraction*, 3rd Edition, Pearson.

MCH-4M4: Emerging Materials and Device Applications

Semester	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-4M1	2	50 (UE=30, IA=20)	Material Special (DSE)

Objective

To provide an advanced understanding of the design, synthesis, functionalization and applications of nanomaterials for sustainable energy, environmental remediation, sensing and biomedical technologies.

Unit I: Nanomaterials for Energy, Sensing and Biomedical Applications

Nanoscopic phenomena and structure–property relationships of nanomaterials. Nanomaterials for energy storage and conversion: lithium-ion, sodium-ion and solid-state batteries; supercapacitors; hybrid energy storage devices; fuel cells and hydrogen storage materials. Nanomaterials for photovoltaics and photocatalysis. Perovskite solar cells and quantum-dot solar cells. Nanomaterials for chemical sensors, gas sensors, biosensors, electrochemical sensors, optical sensors and surface plasmon resonance (SPR)-based sensing. Biomedical applications of nanomaterials: drug delivery systems, nanocarriers, magnetic nanoparticles for hyperthermia, bioimaging, tissue engineering, theranostics and neuroelectronic interfaces.

Unit II: Nano-enabled Technologies for Water and Environmental Applications

Nanotechnology for water treatment and environmental remediation. Sources and types of water pollutants. Adsorption mechanisms (adsorption isotherms and kinetics). Nanomaterials for advanced oxidation processes (AOPs): TiO_2, ZnO, g-C_3N_4, Fenton and photo-Fenton catalysts. Electrochemical wastewater treatment. Membrane technologies: nanofiltration, ultrafiltration, reverse osmosis and nanocomposite membranes. Nanomaterials for desalination and water purification. Nanosensors for water quality monitoring. Internet of Things (IoT)-enabled smart environmental monitoring systems. Solar-driven water purification, magnetic separation technologies and integrated hybrid treatment systems.

Essential Reading

1. Getnet, M., Yirak, Y. and Chaujar, R., *Fundamentals of Emerging Nanomaterials*, Elsevier.
2. Song, Y., Thoutam, L. R., Tayal, S., Balmukund Rahi, S., Samuel, T. S. A., *Handbook of Emerging Materials for Semiconductor Industry*, Springer.
3. Okpara, C. E., Quadri, T. W., Verma, C., Ekpo, S. C., Onwudiwe, D. C. and Banks, C. E. (Eds.), *Handbook of Perovskites: Chemistry, Synthesis and Applications*, Elsevier.
4. Falcon, R., *Handbook of Nanomaterials*, CRC Press.
5. Zarzycki, P. K. (Ed.), *Pure and Functionalized Carbon-Based Nanomaterials: Analytical, Biomedical, Civil and Environmental Engineering Applications*, CRC Press.
6. Cao, G. and Wang, Y., *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, 2nd Edition, World Scientific.
7. Poole, C. P. Jr. and Owens, F. J., *Introduction to Nanotechnology*, Wiley–Interscience.
8. Rai, M. and Duran, N. (Eds.), *Metal Nanoparticles in Microbiology*, Springer.