Postgraduate Papers in Chemistry

EFFECTIVE FROM JULY 2024

M.Sc. CHEMISTRY (M26)

PAPERS: CORE, SPECIALIZATION, ELECTIVE, SKILL ENHANCEMENT (SEC), ABILITY ENHANCEMENT (AEC)

Department of Chemistry
Faculty of Sciences
Jamia Millia Islamia
(A Central University by Act of Parliament)
Jamia Nagar, New Delhi-110025

Course Structure for M.Sc. Chemistry (Effective 2024–25)
(Paper Types: Core, AEC, SEC, Specialization, Elective)

Semester-wise Distribution of Papers in M.Sc. Chemistry

Sem	Paper Code	Paper Title	Paper Type	Credits (Marks)
I	MCH-101	Inorganic Chemistry-I	Theory (Core)	3 (100)
	MCH-101L	Inorganic Chemistry Practical-I	Practical (Core)	1 (50)
	MCH-102	Elements of Materials Chemistry-I	Theory (Core)	3 (100)
	MCH-102L	Elements of Materials Chemistry Practical-I	Practical (Core)	1 (50)
	MCH-103	Stereochemistry and Reactive Intermediates	Theory (Core)	3 (100)
	MCH-103L	Organic Chemistry Practical-I	Practical (Core)	1 (50)
	MCH-104	Thermodynamics & Statistical Thermodynamics	Theory (Core)	3 (100)
	MCH-104L	Physical Chemistry Practical-I	Practical (Core)	1 (50)
	MCH-105	Group Theory and Spectroscopy	Theory (Elective)	4 (100)
		Total Credits (Marks) in Semester I		**20 (700)**
II	MCH-201	Inorganic Chemistry-II	Theory (Core)	3 (100)
	MCH-201L	Inorganic Chemistry Practical-II	Practical (Core)	1 (50)
	MCH-202	Elements of Materials Chemistry-II	Theory (Core)	3 (100)
	MCH-202L	Elements of Materials Chemistry Practical-II	Practical (Core)	1 (50)
	MCH-203	Pericyclic Reactions and Photochemistry	Theory (Core)	3 (100)
	MCH-203L	Organic Chemistry Practical-II	Practical (Core)	1 (50)
	MCH-204	Macromolecules & Surface Chemistry	Theory (Core)	3 (100)
	MCH-204L	Physical Chemistry Practical-II	Practical (Core)	1 (50)
	MCH-205	Interpretative Spectroscopy	Theory (Elective)	4 (100)
	MCH-206	Mathematical & Computational Methods in Chemistry	Skill Enhancement	4 (100)
		Total Credits (Marks) in Semester II		**26 (800)**
III	MCH-301	NMR Spectroscopy and Lanthanide Shift Reagents	Inorganic Special	3 (100)
	MCH-302	Inorganic Reaction Mechanisms	Inorganic Special	3 (100)
	MCH-303	Organometallic Chemistry-I	Inorganic Special	3 (100)
	MCH-304	Bio-inorganic Chemistry-I	Inorganic Special	3 (100)
	MCH-317	Chemistry of Synthetic and Natural Materials-I	Theory (Elective)	4 (100)
	MCH-318	Environmental and Green Chemistry	Ability Enhancement	4 (100)
	MCH-IL	Inorganic Chemistry Practical-III	Inorganic Special Practical	4 (100)
		Total Credits (Marks) in Semester III for Inorganic Branch		**24 (700)**
III	MCH-305	Conventional Ceramics	Material Special	3 (100)
	MCH-306	Basic Concepts of Crystallography & Crystal Structures	Material Special	3 (100)
	MCH-307	Polymer Chemistry & Technology	Material Special	3 (100)
	MCH-308	Chemistry of Advanced Materials	Material Special	3 (100)
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Sem	Paper Code	Paper Title	Paper Type	Credits
	MCH-317	Chemistry of Synthetic and Natural Materials-I	Theory (Elective)	4 (100)
	MCH-318	Environmental and Green Chemistry	Ability Enhancement	4 (100)
	MCHML	Material Chemistry Practical-III	Material Special Practical	4 (100)
		Total Credits (Marks) in Semester III for Material Branch		**24 (700)**
III	MCH-309	Methods in Organic Synthesis	Organic Special	3 (100)
	MCH-310	Advance Tools in Organic Synthesis	Organic Special	3 (100)
	MCH-311	Asymmetric Synthesis & Disconnection Approach in Organic Synthesis	3 (100)	
	MCH-312	Chemistry of Heterocyclic Compounds	Organic Special	3 (100)
	MCH-317	Chemistry of Synthetic and Natural Materials-I	Theory (Elective)	4 (100)
	MCH-318	Environmental and Green Chemistry	Ability Enhancement	4 (100)
	MCHOL	Organic Chemistry Practical-III	Organic Special Practical	4 (100)
		Total Credits (Marks) in Semester III for Organic Branch		**24 (700)**
III	MCH-313	Advanced Statistical Mechanics	Physical Special	3 (100)
	MCH-314	Advanced Solid State Chemistry	Physical Special	3 (100)
	MCH-315	Chemical Kinetics	Physical Special	3 (100)
	MCH-316	Quantum Chemistry	Physical Special	3 (100)
	MCH-317	Chemistry of Synthetic and Natural Materials-I	Theory (Elective)	4 (100)
	MCH-318	Environmental and Green Chemistry	Ability Enhancement	4 (100)
	MCHPL	Physical Chemistry Practical-III	Physical Special Practical	4 (100)
		Total Credits (Marks) in Semester III for Physical Branch		**24 (700)**
IV	MCH-401	Chemical Applications of Group Theory	Inorganic Special	3
	MCH-402	Stereochemistry and Metal Ion Catalysis	Inorganic Special	3 (100)
	MCH-403	Organometallic Chemistry-II	Inorganic Special	3 (100)
	MCH-404	Bio-inorganic Chemistry-II	Inorganic Special	3 (100)
	MCH-417	Chemistry of Synthetic and Natural Materials-II	Theory (Elective)	4 (100)
	M.Sc. Project*	Project Work	Inorganic Special Project	4 (200)
		Total Credits (Marks) in Semester IV for Inorganic Branch		**20 (700)**
IV	MCH-405	Technical Ceramics	Material Special	3
	MCH-406	Processing and characterization of Crystal Structures	Material Special	3 (100)
	MCH-407	Polymer Technology, Processing and Specialty Polymers	Material Special	3 (100)

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Sem	Paper Code	Paper Title	Paper Type	Credits
	MCH-408	Properties of Materials	Material Special	3 (100)
	MCH-417	Chemistry of Synthetic and Natural Materials-II	Theory (Elective)	4 (100)
	M.Sc. Project*	Project Work	Material Special Project	4 (200)
		Total Credits (Marks) in Semester IV for Material Branch		**20 (700)**
IV	MCH-409	Medicinal Chemistry and Biomolecules	Organic Special	3
	MCH-410	Advanced Methods in Organic synthesis	Organic Special	3 (100)
	MCH-411	Chemistry of Natural Products	Organic Special	3 (100)
	MCH-412	Applications of Spectroscopy	Organic Special	3 (100)
	MCH-417	Chemistry of Synthetic and Natural Materials-II	Theory (Elective)	4 (100)
	M.Sc. Project*	Project Work	Organic Special Project	4 (200)
		Total Credits (Marks) in Semester IV for Organic Branch		**20 (700)**
IV	MCH-413	Advance Molecular spectroscopy	Physical Special	3
	MCH-414	Nano Chemistry	Physical Special	3 (100)
	MCH-415	Advance Physical Chemistry	Physical Special	3 (100)
	MCH-416	Electrochemistry	Physical Special	3 (100)
	MCH-417	Chemistry of Synthetic and Natural Materials-II	Theory (Elective)	4 (100)
	M.Sc. Project*	Project Work	Physical Special Project	4 (200)
		Total Credits (Marks) in Semester IV for Physical Branch		**20 (700)**

*PROJECT WORK IN SEMESTER-IV

- The students of Semester-IV shall be allotted Research based project work under the supervision of the concerned faculty member in their respective discipline.
- The entire project work shall include Literature Survey, Experimental Procedures, and Characterization of the synthesized Compounds followed by compilation of Results as Project dissertation work.
- They shall submit a project dissertation towards the semester end, which shall be evaluated by an external expert and internal examiners followed by the presentation/ viva voce.

MCH-101: INORGANIC CHEMISTRY-I

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
I	MCH-101	I	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Metal Ligand Equilibria in Solution 12 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: Non–Aqueous Solvents 12 L

Role of solvents in chemical reactions, physical properties of a solvent, types of solvent and their general characteristics. Reactions in non-aqueous solvents with reference to liquid ammonia and liquid sulfur dioxide (SO_2).

Unit III: Magnetic Properties of Transition Metal Complexes 14 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, superparamagnetism. High and low spin equilibria, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Unit IV: Inorganic Materials 12 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, ICs, 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 (1976).
2. Hartley, F. R., Burgess, C. & Alcock, R. M. *Solution Equilibria*, Prentice-Hall, Europe (1980).
3. Ringbom, A. *Complexation in Analytical Chemistry*, Wiley, New York (1963).
4. Sisler, H. H. *Non-aqueous Solution Chemistry.*
5. Carlin, R. L. *Magnetochemistry.*

Suggested Reading

1. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes*, Chapman and Hall, U.K. (1973).
2. Keer, H. V. *Principles of the Solid State*, Wiley Eastern Ltd., New Delhi (1993).
3. West, A. R. *Solid State Chemistry and its Applications*, John Wiley & Sons (1987).
4. Cheetham, A. K. & Day, P. (Eds.) *Solid State Chemistry Techniques*, Clarendon Press, Oxford (1987).

MCH-101L: INORGANIC CHEMISTRY LAB-1

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-101L	1	50 (UE=25, IA=25)	Practical (Core)

1. Synthesis and Characterization of Complexes Preparation of the following inorganic compounds and their characterization using IR, electronic spectra, Mössbauer and ESR spectroscopy:
   (a) $VO(acac)_2$
   (b) Cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
   (c) $Na[Cr(NH_3)_2(SCN)_4]$
   (d) $K_3[Fe(C_2O_4)_3]$
2. Quantitative Analysis Separation and determination of two metal ions 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 nitrite in water by colorimetric method

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. Scaff, *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: ELEMENTS OF MATERIALS CHEMISTRY-I

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
I	MCH-102	II	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Glasses **8 L**

General features, fabrication of glass, factors affecting glass formation: viscosity; electronegativity; bond types. Theories of glass formation: Zachariasen's Rule, Sun and Rawson Criteria; thermodynamics of glass formation; methods of glass formation. Various types of glasses and their properties: Pyrex glass; Vycor glass; phosphate glasses, borate glasses, chalcogenide glasses.

Unit II: Multiphase Materials **12 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 rules; 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: Polymeric Materials **14 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, superparamagnetism. High and low spin equilibria, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Unit IV: Nanomaterials **14 L**

Nano-scale regime. Types of nanomaterials: nanoparticle, nanoporous; gas-phase nanoparticles; condensed phase nanoparticles; inorganic nanoparticles. Methods of preparation: bottom-up and top-down approaches; reduction methods; sol-gel methods; co-precipitation method; zeolite method; emulsion method. Properties of nanoparticles: physical, mechanical, chemical, magnetic, optical and electronic properties.

Essential Reading

1. A. R. West, *Introduction to Solid State Chemistry*
2. W. D. Callister, *Materials Science and Engineering: An Introduction*, Wiley
3. F. W. Billmeyer, *Textbook of Polymer Science*
4. R. J. Young and P. A. Lovell, *Introduction to Polymers*

Suggested Reading

1. Harry R. Allcock, *Introduction to Materials Chemistry*
2. Mark Weller, *Inorganic Materials Chemistry*
3. H. V. Keer, *Principles of Solid State*, Wiley Eastern
4. Leonard V. Interrante and M. J. Hampden-Smith, *Chemistry of Advanced Materials*
5. G. Challa, *Polymer Chemistry*

MCH-102L: ELEMENTS OF MATERIALS CHEMISTRY LAB-1

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-102L	1	50 (UE=25, IA=25)	Practical (Core)

1. Analysis of Steel Sample
   (a) To determine the percentage of manganese in the given sample of steel.
   (b) To determine the percentage of phosphorus in the given sample of steel.
   (c) To determine the percentage of sulphur in the given sample of plain carbon steel.
   (d) To determine the percentage of silicon in the given sample of plain carbon steel.
2. Analysis of Brass Sample
   (a) To determine the percentage of tin in the given sample of brass.
   (b) To determine the percentage of lead in the given sample of brass.
   (c) To determine the percentage of copper in the given sample of brass.
   (d) To determine the percentage of zinc in the given sample of brass.
3. Synthesis of Polymers
   (a) To prepare polystyrene by bulk polymerization method and report the yield and solubility.
   (b) To determine the molecular weight of the prepared polystyrene by viscometry.
   (c) To determine the molecular weight of commercial polystyrene by viscometry and compare the molecular weights of the prepared and commercial polystyrene.

Reference Book:

1. *Laboratory Manual prepared by the Teacher–in–Charge*

MCH-103: STEREOCHEMISTRY & REACTIVE INTERMEDIATES

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
I	MCH-103	III	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Configurational Isomerism 8 L

Stereoisomerism: classification, optical activity and chirality, resolution of racemic mixture, molecules with one, two or more chiral centers; Fischer's projection formula, relative and absolute configurations, D/L, R/S, and E/Z systems of naming. Stereochemistry due to the presence of perpendicular dissymmetric planes in allenes, spiranes, biphenyls, binaphthols & adamantane. Chirality due to helical shape and chirality due to chiral plane. Optical purity, percentage enantiomeric excess (ee), enantiotopic and diastereotopic atoms, groups and faces. The Felkin–Anh, Hauk and Cornforth models; Cram's and Prelog's rules.

Unit II: Aromaticity and Principles of Reactivity 12 L

Alternant and non-alternant hydrocarbons; Frost circle diagrams and consequences of aromaticity; Hückel's, Craig's and Clair's rules; Homo-, Quasi-, Dual-, Y-type, Möbius- and Baird-type aromaticity. Aromaticity in benzenoid and non-benzenoid systems including annulenes, fulvenes and fulvalenes. HMO approach to compare the aromatic nature of the compounds and NMR interpretation in aromatic and anti-aromatic systems.
Transition state theory, kinetic vs thermodynamic stability of products, potential energy diagrams and Hammond's postulate, Curtin–Hammett/Winstein–Holness kinetics, Marcus relation. Methods of elucidating reaction mechanisms: kinetic and non-kinetic methods, stereochemical evidence, crossover experiments, isotopic effects. Linear free energy relationships: Hammett equation — significance of σ, σ^+, σ^- and ρ; Taft equation, Swain–Scott equation, Winstein–Grunwald equation.

Unit III: Conformational Analysis 8 L

Conformation in open-chain systems; conformational analysis of cyclopentane, cyclohexane, decalins, perhydroanthracene, perhydrophenanthrene, sugars, steroids, and rings containing sp^2 hybridized carbon atoms. Baeyer's strain theory of cyclic compounds, and effect of conformation on reactivity. Fürst–Plattner and alpha-halo rules.

Unit IV: Reactive Intermediates 14 L

Carbocations: Classical and nonclassical carbocations, neighboring group participation, stability and reactivity of bridgehead carbocations. Bredt's rule.
Carbanions: Stability and structure; generation and fate of organometallic compounds; ambident ions and their general reactions. HSAB principle and its applications.
Free radicals: Stability and structure, generation and fate of free radicals, memory and captodative effects; radical ions.
Other intermediates: Generation, structure and reactions of carbenes, nitrenes, benzynes.

Essential Reading

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. Bruckner, R., *Advanced Organic Chemistry*, Elsevier (2002).

7. Addy Pross, *Theoretical and Physical Principles of Organic Reactivity* (1995).

Suggested Reading

1. P. S. Kalsi, *Organic Reactions, Stereochemistry and Mechanisms*, Fourth Edition, New Age International Publishers (2006).

2. E. L. Eliel, *Stereochemistry of Carbon Compounds*, Textbook Publishers (2003).

3. R. Bruckner, *Advanced Organic Chemistry*, Elsevier (2002).

MCH-103L: ORGANIC CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-103L	1	50 (UE=25, IA=25)	Practical (Core)

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 (TLC), and column chromatography.
2. Separation of a Binary Mixture Separation of a binary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis.
3. Separation of a Ternary Mixture Separation of a ternary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis.
4. Preparations of the Following Compounds
   (a) 4-Iodonitrobenzene
   (b) Hippuric acid
   (c) Sorbic acid
   (d) Methyl orange
   (e) Fluorescein
   (f) Oil of wintergreen
   (g) Benzimidazole
   (h) BINOL

Reference Book:

1. *Comprehensive Practical Organic Chemistry* by V.K. Ahluwalia
2. *Monograph on Green Chemistry Laboratory Experiments*, Green Chemistry Task Force Committee, DST
3. *Advanced Practical Organic Chemistry* by N.K. Vishnoi

MCH-104: THERMODYNAMICS & STATISTICAL THERMODYNAMICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
I	MCH-104	IV	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Basic Thermodynamics **4 L**

Overview of the laws of thermodynamics; fundamental concepts of entropy and residual entropy; temperature dependence of free energy; thermodynamic equilibria and associated free energy functions; physical equilibria involving phase transitions; and Maxwell's thermodynamic relations.

Unit II: Equilibrium Thermodynamics **11 L**

Partial molar quantities: partial molar free energy, volume, and heat content—their definitions and significance. Methods for determining partial molar properties. Chemical potential and related thermodynamic functions; variation of chemical potential with temperature and pressure; chemical potential in ideal gas mixtures. Thermodynamic functions of mixing; concept and determination of fugacity. Non-ideal systems: excess thermodynamic functions and their interpretation. Gibbs-Duhem and Margules equations and their applications.

Unit III: Irreversible Thermodynamics **12 L**

Thermodynamic criteria for non-equilibrium states; foundational postulates and methodologies. Onsager's theory and phenomenological laws and equations; transformation of generalized fluxes and forces; principle of microscopic reversibility and Onsager's reciprocal relations. Concepts of entropy production and entropy flow; the theorem of minimum entropy production. Applications to chemical reactions, coupled processes, and electrokinetic phenomena.

Unit IV: Statistical Thermodynamics **18 L**

Microstates and macrostates; statistical distribution concepts including binomial and multinomial distributions for both non-degenerate and degenerate systems; thermodynamic probability and the most probable distribution. Principles of ensemble theory and averaging, covering canonical, microcanonical, and grand canonical ensembles; the significance of molecular and assembly partition functions in statistical thermodynamics. Derivation of distribution laws using Lagrange's undetermined multipliers and Stirling's approximation. Overview of Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. Calculation of thermodynamic properties of ideal gases using partition functions, along with the statistical interpretation of entropy. Treatment of ortho- and para-hydrogen in terms of statistical weights and symmetry number. Determination of equilibrium constants for gaseous reactions using partition functions and the treatment of perfect gas mixtures. Einstein and Debye models for the heat capacities of monatomic solids and their thermodynamic implications.

Essential Reading

1. *An Introduction to Chemical Thermodynamics*, R. P. Rastogi and R. R. Mishra, Vikas Publishing House Pvt. Ltd.
2. *Physical Chemistry*, P. W. Atkins, ELBS.
3. *Statistical Thermodynamics*, M. C. Gupta, New Age International.
4. *Thermodynamics*, J. Rajaram and J. C. Kuriacose, Educational Publishers.

5. *Statistical Mechanics*, Donald A. McQuarrie, Viva Books Pvt. Ltd., New Delhi, 2003. (530.13 MCQ 270916)

Suggested Reading

1. *Thermodynamics*, R. C. Srivastava, Subit K. Saha, Abhay K. Jain, Prentice Hall of India Pvt. Ltd.

2. *Statistical Physics (Part)*, Course of Theoretical Physics, Vol. 5, L. D. Landau and E. M. Lifshitz, Pergamon Press, London.

3. *Physical Chemistry*, T. Engel and P. Reid, Pearson Education and Dorling Kindersley (India), 2006.

4. *Elements of Statistical Thermodynamics* (2nd Edition), Leonard K. Nash, Addison Wesley, 1974. (541.369 NAS X639)

5. *Physical Chemistry: Statistical Mechanics*, Horia Metiu, Taylor & Francis, 2006. (530.13 MET 276461)

6. *Statistical Thermodynamics*, B. J. McClelland, Chapman and Hall & Science Paperbacks, London, 1973. (536.7 MCC 37251)

MCH-104L: PHYSICAL CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
I	MCH-104L	1	50 (UE=25, IA=25)	Practical (Core)

1. Determine the percentage composition of a liquid mixture by viscosity method.
2. Determine the radius of sucrose molecule by viscosity method.
3. Determine molar surface energy of ethyl alcohol by surface tension.
4. To find out composition of a solution by surface tension measurement.
5. Find out molar surface area as a function of concentration for n-propyl alcohol and n-butyl alcohol over water.
6. Verify the law of refraction for mixtures, using glycerol and water.
7. Determine the formation of compounds between two liquids in the mixture.
8. Study the saponification of ethyl acetate by sodium hydroxide solution.
9. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
10. Determine the specific reaction rate of the potassium persulphate–iodide reaction by initial rate method.
11. Study the kinetics of the iodination of acetone in the presence of acid by the initial rate method.
12. Study the adsorption of oxalic acid on charcoal.
13. Determine the heat of neutralization of hydrochloric acid and sodium hydroxide.
14. Determine the heats of reaction for the following:
    (i) $CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$
    (ii) $HC_2O_4^- + H_2O \rightarrow H_2C_2O_4 + OH^-$
15. Find out the dimerization constant of benzoic acid in benzene by titration method.
16. Construct the phase diagram of water–ethanol–benzene system.
17. Find out the molar mass of succinic acid by partition method.

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. *Laboratory Manual of Physical Chemistry*, S. K. Sharma and Arun Sharma, Ane Books.
6. *Instrumental Methods of Chemical Analysis*, B. K. Sharma, Goel Publishing House.
7. *Physical Chemistry: A Laboratory Manual*, Rajan Katoch, Universities Press.
8. *Experimental Physical Chemistry – A Laboratory Textbook*, V. D. Athawale and Parul Mathur, New Age International.

MCH-105: GROUP THEORY AND SPECTROSCOPY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
I	MCH-105	V	4	100 (UE=60, IA=40)	Theory (Elective)

Unit I: Symmetry and Group Theory – I 12 L

Symmetry elements and operations. Definition of a symmetry operation. Definition of a symmetry element. Symmetry planes and reflection. The inversion centre. Proper axes and proper rotations. Improper axes and improper rotations. Identity. Products and symmetry operations. Defining properties of a group. Abelian group. Symmetry operations as group elements (Multiplication table). Symmetry point group (Schoenflies notations). Classes of symmetry, operations. Equivalent symmetry elements and atoms.

Unit II: Symmetry and Group Theory – II 12 L

Character tables for C_{2v} and C_{3v} point groups (Construction not required). Representation reducible and irreducible, analysis of reducible representation. Simple Applications of the character table.

Unit III: Electronic Spectroscopy Fundamentals 10 L

Atomic Spectroscopy: The energies of atomic orbitals; Hydrogen atom spectrum; Orbital and spin angular momenta, total angular momentum; the fine structure of hydrogen atom spectrum; the spectra of alkali metal atoms. The spectra of complex atoms: Singlet and triplet states; Spin-orbit coupling; Term Symbols and selection rules.

Unit IV: Electronic Spectroscopy of Polyatomic Molecules 15 L

Energy levels of molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck–Condon principle, electronic spectra of polyatomic molecules. Electronic spectra of transition metals. Emission spectra: radiative and non-radiative decay, internal conversion, spectra of transition, metal complexes, charge-transfer spectra.

Essential Reading

1. Modern Spectroscopy, J.M. Hollas, John Wiley & Sons (2004).
2. Applied Electronic Spectroscopy for Chemical Analysis, Ed. H. Windawi and F. L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders.
5. Chemical Applications of Group Theory, F.A. Cotton.

Suggested Reading

1. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (1962).
2. Basic Principles of Spectroscopy, R. Chang, McGraw Hill, N.Y. (1970).
3. Modern Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, and IBH-Oxford.
4. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell and E.M. McCash.

MCH-201: INORGANIC CHEMISTRY-II

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
II	MCH-201	VI	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Electronic Spectra of Transition Metal Complexes 12 L

Spectroscopic ground states, correlation, crystal field theory and splitting in Oh, Td, 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 method for assignment of absolute configuration in optically active metal chelate and their stereochemical information.

Unit II: Stereochemistry and Bonding in Main Group Compounds 10 L

VSEPR, Walsh diagram (tri- and penta-atomic molecules), dπ–pπ bonds, Bent rule and energetic of hybridization, simple reactions of covalently bonded molecules.

Unit III: Isopoly and Heteropoly Acids and Salts 08 L

Isopolymolybdates, isopolytungstates, isopolyvanadates, heteropoly anions, organo heteropolyanions and heteropoly blues.

Unit IV: Metal Clusters 12 L

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

Suggested Reading

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

MCH-201L: INORGANIC CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-201L	1	50 (UE=25, IA=25)	Practical (Core)

1. **Qualitative Analysis**
   (a) Less common metal ions – Tl, Mo, Ti, Zr, Th, V and U (Two metal ions in cationic/anionic forms).
   (b) Insoluble oxides, sulphates and halides.
2. **Chromatography: Separation of cations and anions by**
   (a) Paper chromatography.
   (b) Column chromatography – ion exchange.
3. **Synthesis and Characterization of Complexes**
   Synthesis of the following inorganic compounds and their studies by IR, electronic spectra, Mössbauer and ESR spectra:
   (a) $[Co(Py)_2Cl_2]$
   (b) $[Ni(NH_3)_6]Cl_2$
   (c) $[Cu(NH_3)_4]SO_4 \cdot H_2O$
   (d) Lanthanide complexes
4. **Spectrophotometric Determination**
   (a) Cu in a brass sample by spectrophotometer
   (b) Nitrate in water sample by colorimetric method
   (c) Ca and Mg in milk and egg
5. **Sodium and potassium by flame photometric method**

Reference Books:

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge.
2. Inorganic Synthesis, McGraw Hill.
3. Handbook of Preparative Inorganic Chemistry Vol. I and II, Academic Press.
4. Standard Methods of Chemical Analysis by W.W. Scaff, Technical Press.
5. Vogel's Qualitative Inorganic Analysis (Revised), Orient Longman.
6. Vogel's Textbook of Quantitative Inorganic Analysis (Revised), J. Besset, R.C. Denny, G.H. Jeffery, and J. Mendhan, ELBS.

MCH-202: ELEMENTS OF MATERIALS CHEMISTRY-II

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
II	MCH-202	VII	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Imperfection in Crystal Lattice 12 L

Types of crystal defects: Points imperfections; Line imperfection; Surface imperfection; Creation of vacancies: Interstitial and Substitutional; 2D imperfections: Edge and Screw dislocation, Twinning, stacking fault, and low and high angle sub-grain boundary. Motion of dislocation, Buerger's vector, effect of dislocation on mechanical properties of materials. Defect Clusters: Extended defects, Split Interstitial, Koch Cluster, Crystallographic shear structure.

Unit II: Phase Transformation and Elastic Deformation 08 L

Time scale for phase changes. Nucleation and Growth, Nucleation Kinetics; Homogeneous and Heterogeneous Nucleation; Growth and overall transformation kinetics. Martensitic transformation, Buerger's classification: reconstructive and displacive transformation. Elastic deformation, Modulus of Elasticity as a parameter of design; Resolved Shear Stress, Relationship of slip and crystal structure of materials; Law of Critical Resolved Shear Stress.

Unit III: Polymers 10 L

Ziegler–Natta co-ordination polymerization, Ring-opening polymerization of ethers, lactones and lactams. Polymers of commercial importance: Polyethylene, Polypropylene, Polyvinyl Chloride, Polystyrene and Polyurethanes. Mass polymerization techniques: suspension and emulsion methods. Mechanical properties of polymers: stress-strain behaviour, tensile strength, elongation at break, Young's modulus and toughness of polymers.

Unit IV: Corrosion 14 L

Classification of corrosion: Chemical corrosion; Electrochemical corrosion. Forms of corrosion: Uniform, Bimetallic, Crevice, Intergranular, Selective Leaching, Pitting, Stress, Erosion, Hydrogen Embrittlement. Cell potential and EMF series, Activation and concentration polarization, Combined polarization, Mixed potential theory, Mixed electrode. High temperature oxide formation, Thermodynamics of high temperature oxide, Pilling–Bedworth ratio, Rate laws of oxidation: Linear, Parabolic and Logarithmic.

Essential Reading

1. Corrosion Engineering by Mars Fontana
2. Material Science and Engineering by Ragavan
3. Materials Science by V. Raghavan

Suggested Reading

1. *Introduction to Solid State Chemistry*, A. R. West
2. *Materials Science and Engineering: An Introduction*, W. D. Callister, Wiley
3. *Text Book of Polymer Science*, F. W. Billmeyer

4. *Principles of Polymerization*, G. Odian

5. *Polymer Science and Technology of Plastics and Rubbers*, P. Ghosh

MCH-202L: ELEMENTS OF MATERIALS CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-202L	1	50 (UE=25, IA=25)	Practical (Core)

1. To prepare polymethyl methacrylate by bulk method and determine its % yield and solubility.
2. To prepare Phenol-Formaldehyde Resins (Resoles and Novolak).
3. To study the kinetics of aqueous corrosion of mild steel by weight loss method—the GMD.
4. To prepare Al_2O_3 by Precipitation Method and determine its density.
5. To study the phase equilibria diagram of Pb-Sn system by direct cooling curve method.
6. To determine the porosity and density of a given ceramic cube.
7. To prepare a copolymer by bulk method and determine its % yield and solubility.

Reference Books

1. Laboratory manuals prepared by Teacher-In-Charge.
2. *A Laboratory Manual of Metals and Alloys* by S. M. Asharaf, Sharif Ahmad and Ufana Riaz.
3. *A Laboratory Manual of Polymers* by S. M. Asharaf, Sharif Ahmad and Ufana Riaz.

MCH-203: PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

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

Unit I: Electrocyclic Reactions **12 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- and 6π-electron systems, torque selectivity (a special kind of selectivity in pericyclic reactions), and pericyclic reactions of ionic species including Nazarov cyclization reaction.

Unit II: Cycloaddition and Sigmatropic Reactions **8 L**

General orbital symmetry rules: [2+2], [2+2+2], [4+2], [6+4], [5+2], [8+2], [14+2] cycloaddition reactions. Cheletropic cycloaddition and cycloreversion reactions. 1,3-dipolar cycloadditions including click chemistry. Sigmatropic reactions: (1,3), (1,5), (1,7), (2,3), (3,3), Ene reaction, Sharpless-Meldal triazole, Studinger reaction, and other group transfer reactions.

Unit III: Basics and Photochemistry of Aromatic Compounds **10 L**

Excited and ground states, singlet and triplet states, forbidden transitions, fate of excited molecules: Jablonski diagram, fluorescence and phosphorescence, determination of photochemical mechanism and quantum yield. Isomerizations, skeletal isomerizations, singlet oxygen reactions. Photo-Fries rearrangement of ethers and anilides. Synthetic applications of Barton and Hofmann–Löffler–Freytag reactions.

Unit IV: Photochemistry of Alkenes and Carbonyl Compounds **14 L**

Cis-trans isomerization, non-vertical energy transfer, photochemical additions, 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; conjugated cyclohexenones. Paterno–Büchi and de Mayo reactions, photooxidation and photoreduction.

Suggested Books

1. Jerry March, *Advanced Organic Chemistry*, Fourth Edition, Wiley & Sons, 2007.
2. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 2004.
3. I. Fleming, *Pericyclic Reactions*, Oxford Science Publications, 1998.
4. Jagdamba Singh and Jaya Singh, *Photochemistry and Pericyclic Reactions*, New Academic Science, 2009.
5. A. Cox and T. Camp, *Introduction to Photochemistry*, McGraw-Hill.
6. N. J. Turro, *Molecular Photochemistry*, Benjamin.

MCH-203L: ORGANIC CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-203L	1	50 (UE=25, IA=25)	Practical (Core)

1. Estimation of glucose, amino group, phenol, and amino acids.
2. Small scale synthesis and purification of the following:
   (a) Succinic anhydride from succinic acid
   (b) Diethyl phthalate from phthalic anhydride
   (c) Acetophenone to oxime
   (d) Anthrone from anthracene
   (e) Fries rearrangement: Phenylacetate
   (f) Mannich reaction
   (g) Cannizzaro reaction
   (h) Aldol condensation
   (i) Diazotization couplings
   (j) Phenolphthalein from phthalic anhydride
3. UV, IR spectra and melting points of simple compounds.

Reference Books

1. A.I. Vogel, *Practical Organic Chemistry.*
2. V.K. Ahluwalia, *Comprehensive Practical Organic Chemistry.*
3. N.K. Vishnoi, *Advanced Practical Organic Chemistry.*

MCH-204: MACROMOLECULES & SURFACE CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
II	MCH-204	IX	3	100 (UE=60, IA=40)	Theory (Core)

Unit I: Surface Phenomenon **08 L**

Surface tension, Capillary action, Surface films (Electro-kinetic phenomenon), Catalytic activity at surfaces. Catalysis on metal surfaces, Metal oxide surfaces. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Unit II: Interfacial Phenomenon **12 L**

Surface active agents, Classification of Surface-active agents, Co-surfactants, Micellization, Microemulsions, Aggregate structures of surfactants, Critical Micellar Concentration, Surfactant packing parameter, Kraft temperature, Factors affecting the CMC of surfactants, Counter ion binding to micelles, Hydrophobic interaction, Thermodynamics of micellization, Mass action models, Solubilization and Phase diagram of ternary microemulsion system.

Unit III: Macromolecules-I **15 L**

Classification and Chain configuration of macromolecules, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Electrically conducting polymers. Polymerization reactions, Kinetics of polymerization, Mechanism of polymerization.
Polymer microstructure: Microstructure based on chemical structure and geometrical structure. Meaning of glass transition temperature (T_g), factors influencing the glass transition temperature, importance of glass transition temperature and molecular weight.

Unit IV: Macromolecules-II **15 L**

Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. 1-D random walk model in detail, Average end-to-end distance.
Properties of an isolated polymer molecule: Ideal chain, Freely-joined Gaussian chain, Distribution of segments in polymer chain, non-ideal chain, excluded volume, Dimension of real chains and scaling laws, Self-avoiding walk.
Concentrated solution and melts: Thermodynamic properties of polymer solutions, concentration fluctuation in polymer solutions, polymer blends, block copolymer.
Molecular motion of polymers in dilute solution: General theory of Brownian motion, Rouse and Zimm Bead spring models, hydrodynamics interactions, dynamic light scattering.

Essential Reading:

1. **Physical Chemistry** 8th Ed., P. W. Atkins and J. De Paula, Oxford University Press, 2006.
2. **Physical Chemistry of Surfaces** – A. W. Adamson, John Wiley & Sons.
3. **Catalytic Chemistry**, Bruce C. Gates, John Wiley & Sons, Inc. 1992.
4. **Catalysis at Surfaces**, I. M. Campbell, Chapman and Hall, New York, 1998.
5. **Terranova, L. Polymer Solutions: Principles and Practice**, John Wiley & Sons Inc. (2002).

6. **Polymer Physics**, M. Rubinstein and R. H. Colby, Oxford University Press (2003).

7. **DEGENNES, P. G.**, *Scaling Concepts in Polymer Physics*, Cornell University Press (1979).

8. **YOUNG, R. J. & LOVELL, P. A.**, *Introduction to Polymers*, 2nd Ed., Chapman & Hall (1991).

Suggested Reading:

1. **Principals of Nanoscience and Nanotechnology**, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.

2. **Nano Science & Technology**, M. A. Shah and Tokeer Ahmad, I. K. International Pvt. Ltd., 2021.

3. **Introduction to Colloid and Surface Chemistry** (2nd Ed.), D. J. Shaw, Butterworths, 1970.

4. **Micelles, Theoretical and Applied Aspects**, Y. Moroi, Plenum Press, New York.

5. **Introduction to Polymer Science**, V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar, Wiley Eastern.

MCH-204L: PHYSICAL CHEMISTRY LAB–I

Semester	Paper Code	Credits	Total Marks	Paper Type
II	MCH-204L	1	50 (UE=25, IA=25)	Practical (Core)

1. Determine the cell constant of the given conductivity cell at room temperature.
2. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's Law of independent migration of ions.
3. Determine the equivalent conductance, degree of dissociation and dissociation constant of acetic acid.
4. Find out strength of weak and strong acids in a given mixture by conductometric titration.
5. Find out solubility and solubility product of the given sparingly soluble salt in water.
6. Find CMC of a given surfactant and, hence, calculate ΔG_{mix} of the surfactant.
7. Verify Debye–Hückel equation for a strong electrolyte in water.
8. Determine the electrode potentials of zinc and copper electrodes in 0.1 M and 0.01 M solutions and calculate E^0 values for these electrodes.
9. Preparation of buffer solution of various pH and determine their pH values.
10. Determination of solubility and solubility product by e.m.f. method.
11. Perform acid-base titration by pH metric method.
12. Find out the first and second ionization constant of H_3PO_4 by pH metric method.
13. Verify Beer–Lambert Law. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a given unknown mixture.

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-205: INTERPRETATIVE SPECTROSCOPY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
II	MCH-205	X	4	100 (UE=60, IA=40)	Theory (Elective)

Unit I: Infrared and Raman Spectroscopy 12 L

Vibrational energies of diatomic molecules, zero point energy, anharmonicity, Morse potential energy diagram. Derivation of selection rules for diatomic molecules based on harmonic oscillator approximation. Dissociation energies from vibrational data. Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Vibrational-rotation spectroscopy, P, Q and R branches. Breakdown of Born–Oppenheimer approximation.

Classical and quantum theories of Raman effect. Stokes and anti-Stokes lines. Polarizability ellipsoids. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules. Mutual exclusion principle. Polarization of Raman lines. Resonance Raman spectroscopy and coherent anti-Stokes Raman spectroscopy (CARS).

Unit II: Electron Paramagnetic Resonance (EPR) Spectroscopy 12 L

Introduction, representation of the spectrum, hyperfine splitting in simple systems. Hyperfine splitting in various structures including methyl radical and bis(salicylaldimine) copper(II). Factors affecting the magnitude of 'g' values. Zero field splitting and Kramers degeneracy.

Unit III: Nuclear Magnetic Resonance (NMR) Spectroscopy 10 L

Basic ideas about instrumentation. Detailed discussion of ^{1}H, ^{13}C, ^{19}F 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 aromatics. Interpretation of NMR spectra of simple compounds.

Unit IV: Mass Spectrometry (MS) 15 L

Principle of mass spectrometry, instrumentation, operation and representation of spectra. Ion production: EI, CI, FD and FAB. Factors affecting fragmentation and ion analysis. Nitrogen rule, Stevenson's rule, effect of isotopes. Mass spectral fragmentation of organic compounds and common functional groups. Molecular ion peak, metastable peak, McLafferty rearrangement. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

References

- J. M. Hollas, *Modern Spectroscopy*, John Wiley & Sons (2004).
- H. Windawi and F. L. Ho (Eds.), *Applied Electronic Spectroscopy for Chemical Analysis*, Wiley Interscience.
- R. V. Parish, *NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry*, Ellis Harwood.
- W. Kemp, *Organic Spectroscopy*, Palgrave.

- D. L. Pavia et al., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India Ed. (2015).
- R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, *Spectrometric Identification of Organic Compounds*, 8th Edition (2014).

MCH-206: MATHEMATICAL & COMPUTATIONAL METHODS IN CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
II	MCH-205	XI	4	100 (UE=60, IA=40)	Skill Enhancement

Unit I: Mathematical Foundations and Linear Algebra 10 L

- **Basic Mathematics:** Algebra (equations, matrices, determinants, number systems, series summations), Geometry (co-ordinate geometry of lines, circles, conic sections), and Calculus (functions, limits, derivatives, Taylor and Maclaurin series).
- **Vectors and Vector Calculus:** Properties of vectors under rotation, scalar and vector triple products, scalar and vector fields, differentiation and integration of vectors, gradient, divergence, curl, Laplacian in Cartesian, spherical polar and cylindrical systems.
- **Operators and Matrices:** Linear and Hermitian operators, commutation relations, ladder operators, recursion relations of Hermite polynomials, Rodrigues's representation, eigenvalues and eigenvectors, Cayley-Hamilton theorem, Gram-Schmidt orthogonalization, diagonalization of matrices.

Unit II: Differential Equations and Multivariable Calculus 8 L

- **Series Expansion and Approximations:** Taylor and binomial series (statements only).
- **Ordinary and Partial Differential Equations:** Linear independence, general and particular solutions, homogeneous equations, power series solutions. First- and second-order ODEs, integrating factor method, Wronskian, initial value problems.
- **Multivariable Calculus:** Partial derivatives, exact and inexact differentials, integrating factors, constrained maxima and minima (Lagrange multipliers).

Unit III: Transforms and Special Functions 12 L

- **Fourier Transformation:** Fourier series, sine and cosine forms, exponential Fourier series, Fourier integrals and transforms, applications in physical chemistry.
- **Laplace Transformation:** Laplace transform and its inverse, solution of initial value problems using Laplace transform.
- **Special Functions:** Legendre and Hermite polynomials, Rodrigues formula, generating functions, recurrence relations, orthonormality and orthogonality relations, applications in solving physical problems.

Unit IV: Basics of C Programming and Numerical Methods 12 L

Basics of C Programming: Elements of C Language. Types of C Constants, Variables, Instructions, inbuilt functions, arithmetic expressions, hierarchy of operations, use of parentheses, modulus operator. C keywords and commands. Control instructions; Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays. File I/O (Input and Output). *Hands on training.*

Numerical Methods: Solution of quadratic equation by formula, Numerical methods for the roots of polynomial equations, numerical differentiation, numerical integration (Trapezoidal

rule, Simpson's rule). Solution of ordinary differential equations, matrix inversion and diagonalization – the Jacobi transformation for the diagonalization of a symmetric matrix.
Application of Numerical Methods to Chemistry.

Essential Reading:

1. G. B. Arfken, H. J. Weber, F. E. Harris, *Mathematical Methods for Physicists*, 7th Ed., Elsevier, 2013.
2. Erwin Kreyszig, *Advanced Engineering Mathematics*, Wiley India.
3. R. G. Mortimer, *Mathematics for Physical Chemistry*, 2nd Ed., Elsevier, 2005.
4. Donald A. McQuarrie, *Mathematics for Physical Chemistry: Opening Doors*, 2008.
5. Free C Compilers for Windows are available at:
   - `http://www.cprogramming.com/code_blocks/`
   - `http://download.savannah.gnu.org/releases/tinycc/`
6. S. K. Srivastava and Deepali Srivastava, *C in Depth*, BPB Publications, 3rd Ed., 2017.
7. Yashavant P. Kanetkar, *Let Us C*, 5th Ed., BPB Publications, 2004.
8. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill, 2011.
9. J. P. C. Isenhour, Thomas L. Wilkins, *Basic Programming for Chemists: An Introduction*, Wiley-Blackwell, 1987.
10. E. Balagurusamy, *Numerical Methods*, Tata McGraw Hill, 2000.
11. V. Rajaraman, *Computer Oriented Numerical Methods*, PHI Learning Pvt. Ltd., 2018.

MCH-301: NMR SPECTROSCOPY AND LANTHANIDE SHIFT REAGENTS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-301	XII(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Lanthanide Complexes of β-Diketones 10L

Introduction: Overview of β-diketone ligands and types of complexes. Synthesis, Structural, Physical and Chemical properties. Volatile β-diketone complexes.

Unit II: Applications of Nuclear Magnetic Resonance Spectroscopy 12L

Applications of spin-spin coupling to structure determination: $Rh(\Phi P_3)_3Cl_3$, Diphosphate anion ($HP_2O_5^{3-}$), SbF_5, Measurement of magnetic susceptibility by NMR., NMR of paramagnetic transition metal ion complexes – Contact and Pseudo contact shifts, Contact shift and Covalency, Contact shifts in coordinated pyridine.

Unit III: Lanthanide Shift Reagents 14L

Historical development and general principles. NMR of paramagnetic lanthanide complexes – Nature of the shift. The lanthanide shift reagents. Relative shifting and broadening abilities of the lanthanides. Hinckley's shift reagent. Effect of increasing coordination number of the lanthanide on the NMR spectra of added substrate.

Unit IV: NMR of Lanthanide Complexes 12L

NMR of dia and paramagnetic lanthanide(III) complexes, Complexes containing N-donor ligands, (b) Complexes of O-donors, (c) Mixed-ligand complexes, (d) Complexes with varying coordinates, (e) Study of NMR spectra of eight and ten-coordinated paramagnetic lanthanide complexes, (f) Shift reagents as structural probes, (g) Effect of aromatic solvents on the spectra of lanthanide complexes.

Essential Reading

1. Physical Methods in Chemistry: by R.S. Drago.
2. NMR of Paramagnetic molecules – Principles and Applications, Edited by LaMar, Horrocks and Holm, Academic Press (N.Y.).

MCH-302: INORGANIC REACTION MECHANISM

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-302	XIII(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Introduction to Inorganic Reaction Mechanism 12 L

Introduction to labile and inert octahedral complexes, interpretation of lability and inertness of transition metal complexes – Valence Bond and Crystal Field theories, factors affecting the lability of complex, transition state or activated complex, substrate, attacking reagents–electrophilic and nucleophilic, types of substitution reactions– nucleophilic or ligand substitution (SN) and electrophilic or Metal substitution (SE) reactions.

Unit II: Mechanism of Substitution Reactions in Octahedral Complexes 12 L

Mechanism of nucleophilic substitution reactions in octahedral complexes SN1 or dissociation and SN2 or association (or displacement) mechanisms, hydrolysis reactions–mechanisms of acid hydrolysis and base hydrolysis, reactions of octahedral Co(III) amine complexes.

Unit III: Mechanism of Substitution Reactions in Square Planar Complexes 14 L

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

Unit IV: Electron Transfer (or Oxidation-Reduction) Reaction 12 L

Electron transfer reactions, mechanism of one-electron transfer reactions–outer sphere and inner sphere mechanisms, two-electron transfer reactions–complimentary and non-complimentary reactions, mechanism of two-electron transfer reactions.

Essential Reading

1. Inorganic Reaction Mechanism – F. Basolo & G. Pearson.
2. Inorganic Reaction Mechanism – J. O. Edwards
3. Langford, H. & Gray, H.B. *Ligand Substitution Processes* W.A. Benjamin

Suggested Reading

1. Selected Topics in Inorganic Chemistry– Malik, Madan & Tuli.
2. Katakis, D. & Gordon, G. *Mechanisms of Inorganic Reactions* John Wiley & Sons: N.Y.(1987).

MCH-303: ORGANOMETALLIC CHEMISTRY - I

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-303	XIV(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Organometallics – Main Group and Transition Elements 12 L

Introduction and classification of organometallic complexes. IUPAC nomenclature for metal–π–complexes, Ziese salt, bonding and structure – stability of metal-alkene complexes. Synthesis of organometallic complexes – 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.

Unit II: Metal Carbonyls 12 L

Structure, π-bonding, bonding modes of CO. Syntheses of metal carbonyls. Reactions of metal carbonyls. Carbonyl anions, cations and hydrides. Colman's reagents. Metal Nitrosyls.

Unit III: Ligands; Alkenes, Alkynes, Alkyl and Aryl Groups with Higher Hapticity 14 L

Models of alkene and alkyne – metal bonding. 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. COT as ligand. Neutral spectator ligands.

Unit IV: Structure Elucidation and IR Spectroscopy of Organometallic Complexes 12 L

Vibrational spectra and its 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 vibration in C=C bonds.

Essential Reading

1. Metallo-organic Chemistry – Anthony J. Pearson, John Wiley & Sons Inc.(1985)
2. Inorganic Chemistry – Principles of Structure & Reactivity, J. E. Huheey, E. A. Keiter & R. L. Keiter, IV Edition (2005)
3. Introduction to metal pi-complex chemistry – M. Tsutsui, M. N. Levy, A. Nakamura, M. Ichikawa and K. Mori, Plenum Press, New York & Heme (1970)
4. Organometallic Chemistry – R. C. Mehrotra & A. Singh, Wiley Eastern Ltd.(2000)

Suggested Reading

1. Advanced Inorganic Chemistry – F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo & Manfred Bochmann, VI Edition, John Wiley & Sons Inc (1999)
2. Principles and applications of organotransition metal chemistry – J. P. Collman, L. S. Hegsdus, J. R. Norton and R. G. Finke, University Science Books (1987)
3. Organotransition Metal Chemistry: From Bonding to Catalysis – John F. Hartwig, (2008)

MCH-304: BIO-INORGANIC CHEMISTRY–I

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-304	XV(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Metal Ions in Biological System 12 L

Occurrence and availability of Inorganic elements in organism, transport and storage of Inorganic elements, Dose response of an element, biological function of inorganic elements, beneficial and toxic elements, essential and trace metals.

Unit II: Metal Storage, Transport and Biomineralization 12 L

Siderophore, phytosidorophores, ferretin, transferrin, hemosiderine, biomineralization, assembly of advanced materials e.g. calcium phosphate, calcium carbonate, iron biominerals.

Unit III: Uptake, Transport and Storage of Inorganic Molecule 14 L

Oxygen transport and storage through hemoglobin and myoglobin, Alternative oxygen transport in lower organisms. Photosynthesis: Photochemistry, absorption spectra of photosynthetic pigments, photophosphorylation – energy conversion process.

Unit IV: Transport and Function of Alkali and Alkaline Earth Metals 12 L

Role of Alkali and alkaline earth metals in neuro sensation. Ion Channels, ion pumps, magnesium catalysis of phosphate, ubiquitous regulatory role of calcium.

Essential Reading

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

Suggested Reading

1. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J. J. Lippard, Wiley.
2. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983).

MCHIL: INORGANIC CHEMISTRY PRACTICAL-III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCHIL	4	100 (UE=50, IA=50)	Practical (Core)

1. **Synthesis of inorganic compounds**
   Preparation of following compounds and their study by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines.

   1.1. Synthesis and thermal analysis of group 2 metal oxalate hydrate.

   1.2. Synthesis of metal acetylacetonate; magnetic, IR, NMR studies.

   1.3. Magnetic moment of $Cu(acac)_2 \cdot 2H_2O$.

   1.4. *Cis*- and *Trans*-$[Co(en)_2Cl_2]$

2. **Spectrophotometric Determination**

   2.1. Mn/Cr/V in steel sample

   2.2. Mo/W/V/U by extractive spectrophotometric method

   2.3. F^- / NO_2^- / PO_4^{3-}

   2.4. Iron-phenanthroline complex: Jobs method of continuous variations.

   2.5. Zr-Alizarin Red-S complex: Mole ratio method.

   2.6. Cu-Ethylenediamine complex: Slope-Ratio Method

3. **Chromatographic Separations**

   3.1. Cd and Zn.

Reference Books:

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

MCH-305: CONVENTIONAL CERAMICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-305	XII(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Functional Ceramics

8 L

General concepts, oxide and non-oxide ceramics – functions and applications; microstructure of ceramics; grain boundaries in ceramics, significance and their types, fabrication of polycrystalline ceramics – general aspect, brief treatment of synthesis of powders, forming processes, hot pressing, hot isostatic pressing

Structural Ceramics and their Properties

Oxide ceramics – classification and general characteristics, non-oxide ceramics classification and general characteristics, general aspects and characteristics of alumina, zirconia, silicon nitride, silicon carbide

Unit II: Ceramic Insulators

12 L

Introduction, general aspects of linear dielectrics; glass – different types of glasses and their characteristics, selection criteria for glass insulators, important glass compositions and their thermal mechanical and electrical characteristics and applications, glass used in treatment of radioactive waste, laser glass, colored glass used in photograph.

Unit III: Ceramic Capacitors

14 L

Significance of capacitors, history of development, ferroelectricity and capacitors, Basic capacitor materials – porcelain and steatite, rutile, barium titanate, solid solutions, fine grained materials, additives, relaxor dielectrics; classification of ceramic capacitors – thick film capacitors, single layer discrete capacitors, multilayer capacitors, Basic multi-layer fabrication methods – lamination, stacking, spray deposition, build up process, electrode alloys; Barrier layer capacitors – composition, fabrication, characteristic, applications; capacitor performance parameters

Unit IV: Aerogel

14 L

Introduction, Production of Aerogels, silica aerogels, organic aerogels, drying, structural investigations – aerogel structure, thermal and infrared optical properties and mechanical properties, applications

Essential Reading:

1. Introduction to Fine Ceramics by Noburu Ichinose (ed.), John Wiley and Sons, New York (1987)
2. Ceramic Materials for Electronics – R.C. Buchanan (ed.), Marcel Deller, New York (1991)
3. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (ed.), Marcel Deller, New York

Suggested Reading:

1. Modern Ceramic Engineering, Properties, Processing and Use in Design, by David W. Richerson, Marcel Deller, New York

MCH-306: BASIC CONCEPTS OF CRYSTALLOGRAPHY & CRYSTAL STRUCTURES

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-306	XIII(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Crystal Lattice and Unit Cell

10 L

Unit cell and Crystal lattices, brief concept of molecular symmetry, concept of Symmetry in crystal systems, Herman Mauguin notation for symmetry elements in crystal systems, representation of screw axis and glide planes, restriction of symmetry elements in crystals systems, representation of lattice planes and directions, Bravais lattices, concept of Miller indices and Weiss indices, hexagonal crystal system, Determination of miller indices in hexagonal systems, planes of form in crystals, zone rule, possible combination of rotational symmetries, determination of d spacing in crystals

Unit II: Point Groups and Space Groups in Crystal Systems

10 L

Point groups in crystals systems, Herman Mauguin notation of point groups in crystal systems, centrosymmetric and non-centrosymmetric point groups, representation of point groups in crystallography, Concept of space groups, structural elucidation of the following space groups: P1, C2, C2/m, P2221, I4i, determination of atomic coordinates and special positions of space groups, systematic absent reflections, space group and crystal structure of perovskite (ABO_3)

Unit III: Packing in Crystals Structures

14 L

Cubic close packing, hexagonal close packing, packing of ions, alloys and molecular structures, atomic coordinates and nomenclature, structural relationships, polyhedral representation of crystal systems, packing of structures in terms of the distribution of tetrahedral sites, octahedral sites and packing ions. Structural elucidation and distribution of interstitial sites in hcp structures: AX type – wurtzite (ZnS), nickel arsenide (NiAs); AX_2 type – rutile (TiO_2), cadmium Iodide (CdI_2). Structural elucidation and distribution of interstitial sites in ccp structures: AX type – rock salt (NaCl), sphalerite (ZnS), AX_2 type – cadmium chloride ($CdCl_2$), antifluorite (Na_2O), fluorite (CaF_2), classification and structures of silicates and spinels

Unit IV: Preparation of Single Crystals

12 L

Czochralski method, Bridgman and Stock Barger method, zone melting, flux method, Verneuil method, vapor phase transport, hydrothermal methods, high pressure hydrothermal methods, vapour phase transport comparison of the different methods, dry high pressure methods, preparation of nanophase single materials by hydrothermal, microwave- and microwave-solvothermal methods, concept of epitaxial growth factors effecting growth of single crystal structures

Essential Reading:

1. Solid State Chemistry by A.R. West (Wiley)
2. Introduction to Crystallography by D. S. Sands and W.A. Benjamin
3. Understanding Solids: The Science of Materials by Richard Tilley (Wiley).

MCHML: MATERIAL CHEMISTRY PRACTICAL-III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCHML	4	100 (UE=50, IA=50)	Practical (Core)

1. Prepare PMMA by suspension polymerization method and determine its molecular weight by viscometry.
2. Prepare polystyrene by emulsion polymerization method and determine its viscosity average molecular weight.
3. Prepare polyvinyl acetate by solution polymerization and synthesize polyvinyl alcohol from the prepared polymer by hydrolysis.
4. Prepare a copolymer of styrene and methylmethacrylate by solution method.
5. Grow single crystals from the aqueous solutions of:
   (a) Potash alum
   (b) Rochelle salt
6. Determine the bulk density, porosity and specific gravity of the sintered clay piece.
7. Determine the band gap energy of Ge and Si crystals.
8. Study the kinetics of high temperature oxidation of mild steel.
9. Synthesize cobalt ferrite ($CoFe_2O_4$) inverse spinel by chemical route.
10. Measure the dielectric constant of Barium titanate, $BaTiO_3$.

Reference Books:

1. Laboratory manual prepared by the Teacher–in–Charge
2. Crystal and crystal growing by Alam Holden and Phylis Singer
3. A laboratory manual of Polymers by S.M. Ashraf, Sharif Ahmad and Ulfana Ria
4. Practical course in Polymer Chemistry by Pinner
5. Experiments in Polymer Chemistry by Billmeyer

MCH-309: METHODS IN ORGANIC SYNTHESIS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-309	XII(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Formation of C–C Single Bonds 8 L

Generation of thermodynamic and kinetic enolates. Alkylation of enolates and enamines, Silyl enol ethers, Conjugate addition reactions of enolates and enamines, Michael addition, Aldol reactions, Evans aldol reaction, Mukaiyama aldol reaction and stereoselective aldol reactions. Baylis–Hillman, Robinson annulation, and Prins cyclization reaction.

Unit II: Formation of C–C Double Bonds 12 L

Phosphorous ylides (Wittig, Horner–Wadsworth–Emmons and Arbusov reactions), Preparation and application of sulphur ylides (Comparison of action and reactivity of phosphorous and sulphur ylides, Corey–Chaykovsky reaction). Preparation and uses of 1,3-dithiane in organic synthesis (umpolung or reversal of polarity), role of silicon in organic synthesis, origin and consequence of alpha effect and beta effect involving silicon compounds. Formation of alkenes: Shapiro, Bamford–Stevens, Julia, Peterson, Petasis, Corey–Winter, McMurry and Ramberg–Backlund olefinations. Alkenes formation using titanium and chromium reagents.

Unit III: Oxidations 8 L

Oxidation of hydrocarbons (alkanes, alkenes, and aromatic hydrocarbons): Selenium dioxide, DDQ, Etard's and related reaction, epoxidation, Sharpless asymmetric epoxidation, kinetic resolution of chiral allylic alcohol, Prevost and Woodward dihydroxylation, Sharpless asymmetric dihydroxylation. Asymmetric amino-hydroxylation. Palladium catalyzed oxidation of alkenes. Oxidation of alcohols: Chromium reagents, oxidation via alkoxysulfonium salts (DCC & Swern oxidation), manganese reagents (MnO_2, PCC, Jones reagent, Collins reagent) and other metal based oxidants (Ag_2CO_3, RuO_4 and $Tl(NO_3)_3$) oxidative cleavage of C–C bonds. Oxidation of alpha, beta–unsaturated ketones.

Unit IV: Reductions 14 L

Catalytic hydrogenation: Of alkenes, alkynes, aromatic compounds, nitrile, oximes and nitro compounds. Heterogeneous and homogeneous catalysis, stereochemistry and mechanism. Induced asymmetry via homogeneous hydrogenation. Reduction by dissolving metals: Of carbonyl compounds, aromatic compounds (Birch reduction), Alkynes and conjugated dienes. Hydride transfer reagents: Aluminium alkoxides (Meerwein–Ponndorf–Verley reduction), Lithium aluminium hydride, sodium borohydride, sodium cyanoborohydride and tri-sec-butylborohydride (DIBAL-H) with chemoselectivity. Enzymatic reductions, hydrogenation via Wilkinson's catalyst.

Essential Reading

1. Smith M. B. & March, J. *Advanced Organic Chemistry*, Sixth Edition, John Wiley & Sons (2007).

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

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

Suggested Reading

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

2. Bruckner, R. *Advanced Organic Chemistry*, Elsevier (2002).

3. Clayden, Greeves, Warren & W. others, *Organic Chemistry*, Oxford University Press (2001).

4. Lowry, T. H. & Richardson, K. S., *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Educational Publishers, Inc. (1981).

MCH-310: ADVANCED TOOLS IN ORGANIC SYNTHESIS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-310	XIII(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Strategic Applications of Named Reactions 14 L

Mitsunobu, Appel, Nef, Henry, Pfitzinger, Ritter, Koch–Haaf, Kulinkovich and related reactions, Stetter, Duff, Chugaev and related reactions, Regitz, Alkyne-Zipper, Simmons–Smith, Sakurai, Corey–Fuchs and related reactions, Dötz and related annulations, Corey–Seebach, Scholl, Buchner, Rubottom, Reformatsky, Mannich, Betti, Bergilini, Kabachnik–Fields, Darzens, Stobbe, Staudinger, Barton (deoxygenation, deamination, olefination and decarboxylation), Vilsmeier–Haack and related reactions, Weiss–Cook, benzoin and acyloin condensations, Parham cyclization, Weinreb ketone synthesis. Steglich, Yamaguchi, Keck, Mukaiyama, and Corey–Nicolaou lactonization. Reissert, Fürstner, Madlung and Bartoli indole syntheses; Knorr, Piloty–Robinson, and Paal–Knorr pyrrole synthesis; Skraup, Doebner, and Pictet–Spengler reactions; Fischer indolization.

Unit II: Rearrangements 12 L

General mechanistic considerations: nature of migration, migratory aptitude, memory effects. Cationotropic and anionotropic rearrangements. Rearrangements involving electron-deficient carbon, nitrogen and oxygen. Detailed mechanisms of: Beckmann, Dakin, Baeyer–Villiger, Stevens, Sommelet–Hauser, Pinacol–Pinacolone, Wagner–Meerwein, Demjanov, Dienone–Phenol, Benzil–Benzilic acid, Favorskii, Arndt–Eistert, Neber, Pummerer, Payne, Curtius, Hoffmann, Lossen, Schmidt, Ireland–Claisen, Perkin, Wittig, Wolff, Smiles, Mislow–Evans, Overman, Carroll, Meisenheimer, Ciamician–Dennstedt, Achmatowicz, Kakis–Kikuchi, Boekelheide, Bergman, von Richter, Julia, Rupe and Meyer–Schuster rearrangements and other aromatic rearrangements.

Unit III: Fragmentations 10 L

Basic concepts of alpha and beta fragmentations. Named reactions related to fragmentations: Grob fragmentation, Beckmann fragmentation, Eschenmoser–Tanabe fragmentation, Marshall fragmentation, Warton fragmentation, Hanessian–Hullar fragmentation, Pummerer fragmentation, and other important fragmentation reactions.

Unit IV: Organometallics in Organic Synthesis 14 L

Basics: hapticity, 18-electron rule and Wade rules, metal clusters, sandwich compounds, fluxional molecules, catalysis. Structure and bonding in metal–alkyl, –aryl, –allyl, cyclopentadienyl and arene complexes. Reactions at metal–carbon (M–C) and metal–hydrogen (M–H) bonds: oxidative addition, insertion, transmetallation and cyclization. Applications: hydroformylation using cobalt octacarbonyl, Monsanto acetic acid process, hydrogenation using Wilkinson's catalyst, Tebbe reagent, Ziegler–Natta polymerization, Ziese's salt, olefin metathesis, Wacker process, Pauson–Khand, Tsuji–Trost allylation, Nicholas reaction, Buchwald–Hartwig amination, Schwartz reaction.

Coupling reactions: A3, Heck, Suzuki, Stille, Sonogashira, Fukuyama, Hiyama, Negishi, Kumada, Chan–Lam, Castro–Stephens, Petasis, Glaser, Eglinton, Hay and Nozaki–Hiyama–Kishi reactions.

Books Suggested

1. Kurti, L. and Czako, B., *Strategic Applications of Named Reactions in Organic Synthesis* (2004).

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

3. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis – An Introduction*, W. H. Freeman and Company (2006).

4. Ajay Kumar, *Organometallic and Bioinorganic Chemistry.*

5. R. C. Mehrotra & A. Singh, *Organometallic Chemistry*, Wiley Eastern Ltd. (2000).

6. P. R. Jenkins, *Organometallic Reagents in Synthesis*, Oxford Science Publications (1992).

7. J. M. Swan and D. C. Black, *Organometallics in Organic Synthesis*, Chapman & Hall.

MCH-311: ASYMMETRIC SYNTHESIS & DISCONNECTION APPROACH IN ORGANIC SYNTHESIS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-311	XIV(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Asymmetric Synthesis: 12 L

Concise introduction to asymmetric synthesis, detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and organo-catalysts with specific examples including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Introduction to domino/tandem/cascade reaction concepts with selected examples.

Unit II: Protecting of the following groups: 12 L

Role of protective groups in organic synthesis, Protection of carbon-carbon double bonds, alcohols (including 1,2 and 1,3-diols), amine, thiol, carbonyl carboxyl groups, phenols and catechols.

Unit III: Disconnection approach to synthesis of organic molecules: 08 L

An introduction to synthons and synthetic equivalents, conversion and interconversion of functional groups, selective reactions (chemo-, region-, and stereoselective), formation of C–C, C–O, C–N bonds.

Unit IV: Disconnection approach: 14 L

Alcohols and carbonyl compounds, consideration of regioselectivity. Alkene synthesis and uses of acetylenes in organic synthesis.
(b) Two Group C–C Disconnection: Diels Alder reaction, 1,3-difunctionalised compounds, α, β-unsaturated carbonyl compounds, 1,5-difunctionalised compounds. Michael addition and Robinson Annulation. Functional group transformations.

Essential Reading:

1. L. F. Fieser and M. Fieser, *Reagents for Organic Synthesis*, Vol. 1-16 (Vol. 1, 1967), Wiley Interscience, New York.
2. M. B. Smith and J. March, *March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure*, 5th ed. (2001), Wiley-Interscience, New York.
3. M. B. Smith, *Organic Synthesis*, McGraw Hill Inc., New York (1995).
4. J. Clayden, N. Greeves, S. Warren, and E. Wothers, *Organic Chemistry*, Oxford University Press, Oxford (2001).

Suggested Reading:

1. R. Bruckner, *Organic Mechanisms: Reactions, Stereochemistry and Synthesis*, Springer (2009).
2. Disconnection approach to organic synthesis – J. S. Jenkins and D. A. Dixon, Chapman and Hall.

MCH-312: CHEMISTRY OF HETEROCYCLIC COMPOUNDS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-312	XV(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Three and four membered heterocycles 12 L

Nomenclature of heterocyclic compounds, reactivity order of various three, membered and four membered heterocycles, Structure, synthesis and reactions, of aziridines, oxiranes, thiranes, and azetidines.

Unit II: Five and six membered heterocycles 12 L

Structure, preparation, properties and reactions of indole, quinoline and isoquinoline. Order of basicity and aromaticity of different heterocycles containing two hetero atoms.

Unit III: Metallo-porphyrins 08 L

Basics, Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, plastocyanin, hemoerytherine, cyanocobalamine, chlorophylls, and Iron-Sulfur proteins.

Unit IV: Metallo-enzymes 14 L

Basics, chymotrypsin, carboxypeptidase, carbonic anhydrase, alcohol, dehydrogenase and aldehyde oxidase. Nitrogenase enzyme and role of Alkali, and Alkaline earth metal ions (Na^+, K^+, Ca^{2+} & Mg^{2+}) in Biological systems.

Essential Reading:

1. T.L. Gilchrist, *Heterocyclic Chemistry*, 3rd Edition (1997), Addison-Wesley Longman Ltd., England.
2. A.R. Katritzky, C.A. Ramsden, J.A. Joule and V.V. Zhdankin, *Handbook of Heterocyclic Chemistry*, 3rd Edition (2010), Elsevier, Oxford, UK.
3. *Heterocyclic Chemistry*, 4th ed. J.A. Joule and K. Mills, Blackwell Publishing, Indian Reprint 2004.
4. *Heterocyclic Chemistry Vol-III*, 1st ed. R. R. Gupta, M. Kumar, V. Gupta.
5. Springer-Verlag, Berlin Heidelberg Publication (2005).
6. *Aromatic Heterocyclic Chemistry*, David T. Davies, 1992, Oxford University.
7. *Bioinorganic Chemistry - A Short Course*; R. M. Roat-Malone; Wiley Interscience, 2003.
8. *Organometallics and Bioinorganic Chemistry* by Ajay Kumar.

Suggested Reading:

1. Inorganic Chemistry by D. F. Shriver and P. W. Atkins.
2. R. K. Bansal, *Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms*, 3rd Edition (1999), New Age International Publishers, New Delhi.
3. P. R. Jenkins, *Organometallic Reagents in Synthesis*, Oxford Science Publ., Oxford (1992).

4. *Organometallics in Organic Synthesis* – J. M. Swan and D. C. Black (Chapman and Hall).
5. *Protective Groups in Organic Synthesis*, Theodora W. Greene & Peter G. M. Wuts.

MCHOL: ORGANIC CHEMISTRY PRACTICAL-I

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCHOL	4	100 (UE=50, IA=50)	Practical (Core)

1. Use of chemistry software like ChemDraw, ChemOffice etc.
2. (a) Isolation of caffeine from tea leaves
   (b) Isolation of piperine from black pepper
   (c) Isolation of lycopene from tomatoes
3. Preparations, isolation and characterizations: (one/two/three-stage).
   - 3.1 Diels-Alder reaction of anthracene with maleic anhydride
   - 3.2 Diels-Alder reaction between furan and maleic acid
   - 3.3 Synthesis of indole from cyclohexanone and phenylhydrazine
   - 3.4 Para-aminoazobenzene from aniline
   - 3.5 Benzophenone → Benzophenone oxime → Benzanilide (Beckmann rearrangement)
   - 3.6 Anthrone from phthalic anhydride
   - 3.7 Benzoin → Benzil → Benzilic acid
   - 3.8 Nitrobenzene → m-dinitrobenzene → m-nitroaniline → m-nitrophenol
   - 3.9 Phthalic anhydride → phthalimide → anthranilic acid
   - 3.10 Eosin from phthalic anhydride
   - 3.11 Glucosazone from glucose
   - 3.12 Methylene blue from dimethylaniline

Reference Books

1. *Vogel Practical Organic Chemistry*
2. *Comprehensive Practical Organic Chemistry* by V.K. Ahluwalia
3. *Advanced Practical Organic Chemistry* by N. K. Vishnoi

MCH-313: ADVANCED STATISTICAL MECHANICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-313	XII(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit-1: Ensembles **12 L**

Grand Canonical Ensemble: Distribution functions in monatomic, one-component systems; Kirkwood–Salsburg integral equation.
Canonical Ensemble: Canonical partition function and ensemble-averaged properties. Derivation and interpretation of distribution and correlation functions based on the canonical probability distribution. Radial distribution function $g(r)$ and its role in determining the thermodynamic properties of fluids. Potential of mean force; superposition and other closure approximations. Integral equation theories: Kirkwood integral equation, Born–Green–Yvon (BGY) hierarchy, Hypernetted Chain (HNC) approximation, and Percus–Yevick (PY) equation.
Applications: Fluid of hard spheres under the superposition approximation; fluid with modified Lennard-Jones molecular interaction potential using the superposition approximation.

Unit-2: Theory of Imperfect Gases **8 L**

Partition functions and cluster integrals, Pressure of gas expressed as a power series in activity. Irreducible cluster integrals, Virial expansion for a gas, Calculation of Virial coefficients of an imperfect gas. Theory of condensation.

Unit-3: Lattice Statistics **12 L**

Ising Model: Nearest-neighbor lattice statistics; thermodynamic quantities and their interconnections. Exact and formal methods of solution.
Computer Simulation: Motivation and applications of computer simulations in statistical mechanics. Intermolecular potentials; introduction to Molecular Dynamics (MD) and Monte Carlo (MC) methods.

Unit-4: Statistical Theory of Liquids—Supercooled and Ionic Liquids **12 L**

Theories of Transport Properties: Overview of transport phenomena; non-Arrhenius behavior of transport properties. Cohen–Turnbull free volume model; configurational entropy model.
Experimental Methods for Structure Determination: Spectroscopic techniques for the study of liquid structure; neutron scattering and X-ray scattering methods.

Recommended Texts:

1. Allen, M. P. & Tildesley, D. J. *Computer Simulations of Liquids*, Oxford Science Publications: Oxford (1987).
2. Hill, T. L. *Statistical Mechanics: Principles and Selected Applications*, Dover Publications Inc.: New York (1987).
3. Landau, L. D. & Lifshitz, E. M. *Statistical Physics Vol. 5, Part 1*, 3rd Ed., Pergamon Press (1980).
4. McQuarrie, D. A. *Statistical Mechanics*, Viva Books Pvt. Ltd.: New Delhi (2003).
5. Bagchi, B. *Statistical Mechanics for Chemistry with a Computer Simulation Approach*, CRC Press (2018).

MCH-314: ADVANCE SOLID STATE CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-314	XIII(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Concepts of Solids **11 L**

Crystalline and Amorphous Solid, Unit cell, Summary of crystal lattices, Reciprocal lattice, Bonding & packing in crystals, Lattice planes, Symmetry elements, Space lattice, Glide planes, Screw Axis, Point groups and notations of 32, 222, mm2 and mmm point groups, space groups and elucidations of representing point groups; viz. Monoclinic C2, Monoclinic C2/m, Orthorhombic p2221 and Tetragonal I41.

Unit II: Crystal Defects and Non-Stoichiometry in Solids **10 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 & 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 forces, Effect of temperature, Magnetic moment calculations, Ferro- 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.

Unit IV: Structures of Solids **8 L**

Perovskite structure (e.g. $CaTiO_3$ and $BaTiO_3$), Spinel structure (e.g. $MgAl_2O_4$), Rutile TiO_2 structure, Rock salt NaCl structure, Sphalerite and Wurtzite structures of ZnS, Ruddlesden-Popper type K_2NiF_4 (e.g. Sr_2TiO_4) and β-K_2SO_4 (e.g. Ba_2TiO_4) structures.

Essential Reading

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

Suggested Reading

1. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, Cambridge University Press.
2. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
3. Principles of the Solid State, H. V. Keer, New Age International Publishers.

4. Solid State Chemistry, D. K. Chakrabarty, New Age International Publishers.

MCH-315: CHEMICAL KINETICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-315	XIV(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Reaction Dynamics **12 L**

Introduction, Collision, Collision diameter, Collision theory, Collision cross section, Opacity function, Differential and total scattering cross section, Potential energy surfaces, Experimental approaches i.e., Molecular beam scattering and state resolved spectroscopic techniques, Stripping and rebound mechanism, State to state kinetics, Harpoon Mechanism.

Unit II: Statistical Theories of Kinetics **14 L**

Postulates and derivation of transition state theory, Thermodynamic formulations of transition state theory, Applications of transition state theory, Unimolecular reaction rate theory (Lindemann–Hinshelwood treatment), Rice–Ramsperger–Kassel (RRK) theory and Marcus's refinement of RRK theory (RRKM), Kinetic and thermodynamic control, Hammond's postulate.

Unit III: Complex Reactions **12 L**

Chain reactions, Oscillatory reactions, Photochemical reactions, Enzyme kinetics: single and double intermediate mechanisms, King–Altman method for working out the kinetics of complex enzyme reactions, Enzyme-catalyzed reactions kinetics (various types of inhibition).

Unit IV: Kinetic Measurements **12 L**

Introduction, Kinetic systems (i.e., Static systems, flow systems, and shock tubes), Description of techniques (i.e., Flash photolysis and laser flash photolysis, Absorption spectroscopy, Laser photolysis / Chemiluminescence, Laser-Induced fluorescence, and Photoionization techniques), Chemical Relaxation Methods, Treatment of kinetic data.

Essential Reading

1. K. J. Laidler, *Chemical Kinetics*, Third Edition, 1987.
2. L. Wilkinson, *Chemical Kinetics.*
3. M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford University Press, 1995.
4. Jeffrey I. Steinfield, Joseph S. Francisco, William L. Hase, *Chemical Kinetics and Dynamics*, 2nd Edition, 1998.

Suggested Reading

1. James H. Espenson, *Chemical Kinetics and Reaction Mechanism*, 2nd Ed., McGraw-Hill, 1995.
2. P. W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th Ed., Oxford University Press, 2006.
3. Santosh K. Upadhyay, *Chemical Kinetics and Reaction Dynamics*, Anamaya Publishers, New Delhi, 2006.

4. J. I. Steinfeld, J. S. Francisco, and W. L. Hase, *Chemical Kinetics and Dynamics*, 2nd Ed., Prentice Hall International, Inc., 1999.

5. L. Arnaut, Sebastiao Formosinho, and Hugh Burrows, *Chemical Kinetics: From Molecular Structure to Chemical Reactivity*, Elsevier, 2007.

MCH-316: QUANTUM CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-316	XV(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Some Exactly Solvable Problems **15 L**

Postulates of Quantum Mechanics. Discussion of the solution of the Schrödinger equation to some model systems viz. free particle, the rigid rotor, the harmonic oscillator and the hydrogen atom (derivation only of eigenvalue in last two problems. The method to find the wave function is only sketched and result is given). Simple discussion of potential barrier (short study).

Unit II: Approximate Methods **11 L**

The Variation theorem, linear variation principle. Time independent Perturbation theory (first order and non-degenerate), second order change of energy non-degenerate (without proof). Applications of variation method and perturbation theory to Helium atom. Only a brief sketch of time dependent perturbation theory. Formula of the Golden rule written down (without proof). Some simple applications indicated (without proof).

Unit III: Angular Momentum, Spin and Electronic Structure **12 L**

Angular momentum operators, Eigen values and eigen functions, addition of angular momenta, 6j and 9j symbols (without proofs), spin, Antisymmetry and Pauli Exclusion Principle. Electronic configuration, atomic state, Russell–Saunders coupling schemes, term separation energies of the pn configuration, magnetic effects; spin orbit coupling and Zeeman splitting, introduction to the method of self-consistent field.

Unit IV: Molecular Orbital Theory **10 L**

Hybridization & valence MO's of H_2O, NH_3 and CH_4. Huckel Molecular Orbital Theory of conjugated systems. Delocalization energy, electron density, bond order. Application of HMO to ethylene, butadiene, cyclopropenyl radical & benzene (only qualitative discussion for benzene).

Essential Reading

1. I. Levine, *Quantum Chemistry*, 5th Ed., Prentice Hall Inc., New Jersey (2000).
2. T. Engel and P. Reid, *Physical Chemistry*, Published by Pearson Education and Dorling Kindersley (India) (2006).
3. Donald A. McQuarrie, *Quantum Chemistry*, Oxford University Press, 1983 (541.28MCQ).
4. A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill Publishing Company New Delhi.
5. Eyring, Walter & Kimball, *Quantum Chemistry*, John Wiley & Sons, Inc., Chapman & Hall Ltd., 1946.

MCHPL: PHYSICAL CHEMISTRY PRACTICAL-III

Semester	Paper Code	Credits	Total Marks	Paper Type
III	MCHPL	4	100 (UE=50, IA=50)	Practical (Core)

1. Determine the molecular weight of the given polymer sample by viscosity method.
2. Determine the ionization constant of acetic acid by conductivity method.
3. Titrate using conductometer a moderately strong acid (salicylic/mandelic acid) by the
   (a) salt-line method
   (b) double alkali method
4. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid against sodium hydroxide conductometrically.
5. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
6. Carry out the following titrations conductometrically:
   (a) Magnesium sulphate against $BaCl_2$ and its reverse titration
   (b) HCl versus NH_4OH
   (c) Sodium oxalate against HCl
7. Determine the rate constant of saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reaction by conductivity method.
8. Find out the rate constant of acid-catalysed hydrolysis of sucrose by polarimeter.
9. Study the rate equation for mutarotation of D-glucose in water using polarimeter.
10. To determine the partial molar volumes of sodium chloride in water by density measurements. (Page 30 – Das & Behra)
11. To find the formula of the copper–ammine complex ion in aqueous solutions by partition method. (Page 108 – Das & Behra)
12. To determine the hydrolysis constant of aniline hydrochloride by partition method. (Page 113 – Das & Behra)
13. Titrate phosphoric acid potentiometrically against sodium hydroxide.
14. Titrate potentiometrically solutions of:
   (a) KCl / KBr / KI;
   (b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
15. Titrate potentiometrically a solution of ferrous ions against $KMnO_4$ / $K_2Cr_2O_7$. Carry out the titration in the reverse order.
16. Determine the solubility and solubility product of an insoluble salt, AgX (X = Cl, Br or I) potentiometrically.
17. Determine the hydrolysis constant of aniline hydrochloride by pH meter.

18. Determine potentiometrically the heat of reaction equilibrium constant and other thermodynamic functions for a given reaction such as:

$$Zn + Pb^{2+} \rightleftharpoons Zn^{2+} + Pb$$

19. Determine the mean ionic activity coefficients of hydrochloric acid solutions at different concentrations by potentiometer.

20. Determine of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO–water mixture) and calculate the partial molar heat of solution.

21. Determine the transport numbers of cations and anions in a solution with a known concentration by Hittorf's method.

22. To determine the degree of ionization of sodium chloride at different concentrations of its aqueous solutions from the depression of freezing point measurements.
(Page 45 – Das & Behra)

23. Estimation of Pb^{2+} and Cd^{2+}/Zn^{2+} and Ni^{2+} ions in a mixture of these ions by polarography.

24. Determination of dissolved oxygen in aqueous solution of organic solvents by polarography.

25. Determine the formula and overall stability constant of lead oxalate complex at 25°C by polarographic method.

26. To determine the rate constant of the acid hydrolysis of acetal by dilatometry at 298.15K.
(Das & Behra)

MCH-317: CHEMISTRY OF SYNTHETIC AND NATURAL MATERIALS-I

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-317	XVI	4	100 (UE=60, IA=40)	Theory (Elective)

Unit I: Superconductors 15 L

Superconductivity and its origin, High temperature superconductors, Meissner effect, London equation, Type I and II superconductors, Isotope effect, Penetration depth and Coherence length, Anisotropy, Heat capacity, Copper pairs, Josephson effect, BCS theory of superconductivity, Hysteresis in superconductors, Organic superconductors.

Unit II: Chemical Biology 12 L

Introduction: What is Chemical Biology and how it differs from Biochemistry; Basics of Biology: Amino acids, and peptides, Sugars-their function and importance. What is PNA and how it differs from DNA and RNA, synthesis of PNA monomer, oligomer and its applications., Microscopy and Spectroscopy in Biology: AFM, SEM, TEM, DLS, ORD, CD, NMR, MS UV-Vis, Fluorescence

Unit III: Analytical Methods 15 L

Analytical Chemistry: Introduction, Classification of Different Analytical Techniques (chemical methods of analysis, electrical methods of analysis, optical methods of analysis, thermal methods of analysis). Criteria for Evaluating the Utility of Analytical Techniques. Evaluation of analytical data (errors, detection and minimization), accuracy, precision. Mean, median, mode, deviation, standard deviation, relative standard deviation, coefficient of variation, precision, Gaussian distribution of data, t-test, Chi-square test.

Unit IV: Metal Complex Sensitizers 12 L

Concept of metal complex sensitizers; electron relay; metal colloidal systems; semiconductor supported metal oxide systems; nitrogen fixation; water photolysis; carbon dioxide reduction

Essential Reading

1. Dobson, Gerrard & Pratt, Foundations of Chemical Biology; Oxford Univ. Press; 2002.
2. Miller & Tanner, Essentials of Chemical Biology: Structure and Dynamics of Biological Macromolecules; Wiley; 2002.
3. Solid State Physics by Lovel, Avery and Vernon

Suggested Reading

1. Waldman & Janning, Chemical Biology: A Practical Course; Wiley-VCH; 2004.
2. Joseph R. Lackowicz, Principles of Fluorescence Spectroscopy; Springer; 2006.

MCH-318: ENVIRONMENTAL AND GREEN CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
III	MCH-318	XVII	4	100 (UE=60, IA=40)	Ability Enhancement

Unit I: Water Chemistry 15L

Water-quality parameters and standards: Physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon (TOC), Total nitrogen, Total sulfur, Total phosphorus and Chlorine.
Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, chromium, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

Unit II: Novel Inorganic Solids 12L

Synthesis and modification of inorganic solids: Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.
Inorganic solids of technological importance: Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – colored solids, white and black pigments. Molecular material and fullerides, molecular materials and chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

Unit III: Nanomaterials 10L

Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures – control of nanoarchitecture – one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites.

Unit IV: Green Chemistry 15L

Introduction. Need for Green Chemistry, Goals of Green Chemistry, Limitations/ Obstacles in the pursuit of the goals of Green Chemistry, Principles of Green Chemistry and Designing a Chemical synthesis.
Future Trends in Green Chemistry: Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; crystal controlled solid state synthesis; Green chemistry in sustainable development.

Suggested Books

1. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).
2. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
3. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
4. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.
5. G. J. Ferraudi, Elements of Inorganic Photochemistry, John Wiley & Sons (1988).

6. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).

7. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).

8. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society (2002).

9. Anastas, P.T. & Warner, J.C. Green Chemistry, Theory and Practice, Oxford University Press, 1998.

MCH-401: CHEMICAL APPLICATIONS OF GROUP THEORY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-401	XVIII(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Symmetry Aspects of Molecular Vibrations 12 L

Introduction, the symmetry of normal vibrations. Determining the symmetry types of the normal modes (Normal mode analyses of water molecule, carbonate ion and N_2F_2).
Contribution of particular Internal Coordinates to normal modes. Symmetry selection rules for fundamental vibrational transitions (Qualitative treatment). The symmetry of group vibrations (a discussion of molecule $Cl_3C\text{-}CH_2\text{-}CH_2\text{-}CCl_3$ to determine vibrational modes of CH_2 group). Use of symmetry considerations to determine the number of active infrared and Raman lines (example SF_4).

Unit II: Symmetry Aspects of Hybrid Orbitals 12 L

Transformations properties of atomic orbitals. Hybrid orbitals for sigma bonds in trigonal planar (BCl_3), tetrahedral (CH_4), square planar $[PtCl_4]^{2-}$ and trigonal bipyramidal (PF_5). Hybridization scheme for pi bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems.

Unit III: Hybrid Orbitals as Linear Combination of Atomic Orbitals 14 L

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 and trigonal bipyramidal dsp^3 non-equivalent hybrid orbitals in PF_5.

Unit IV: The Huckel Molecular Orbital Treatment and Symmetry Simplifications 12 L

The LCAO method and secular equation. The simple Hückel approach in constructing and solving secular determinants for conjugated systems (ethylene, allyl system and butadiene), delocalization energies.
Symmetry simplifications of Hückel Molecular Orbital method (symmetry factoring of secular equation: 1,3-butadiene).
Calculations of electron density, charge density, Bond order and free valence index.

Essential Reading

1. Chemical Applications of Group Theory: by F.A. Cotton.
2. Group Theory and Symmetry in Chemistry: by Lowell H. Hall
3. Symmetry, Orbitals and Spectra: by Milton Orchin and H.H. Jaffe.
4. Physical Methods in Chemistry: by R.S. Drago.
5. Molecular Spectroscopy: by G.M. Barrow, McGraw-Hill.

MCH-402: STEREOCHEMISTRY AND METAL ION CATALYSIS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-402	XIX(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Stereochemical Changes in Octahedral Complexes-I 12 L

Outer sphere orientations, reactions of geometrical and optical isomers S_N1 dissociation or S_N2 displacement mechanisms, stereochemistry of the acid and base hydrolysis of Co(III) complexes, optical inversion reactions of some Co(III) complexes.

Unit II: Stereochemical Changes in Octahedral Complexes-II 12 L

Isomerization reactions of octahedral complexes, recimerization of octahedral Co(III) complexes, salt and solvent effects, photorecimerization.

Unit III: Photochemical Reactions 14 L

Introduction, types of excitation, fate of excited molecules, quantum yield, types of photochemical reactions.

Unit IV: Metal Ion Catalysis 12 L

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

Essential Reading

1. Inorganic Reaction Mechanism - F. Basolo & G. Pearson.
2. Inorganic Reaction Mechanism - J. O. Edwards
3. Langford, H. & Gray, H.B. *Ligand Substitution Processes*, W.A. Benjamin

Suggested Reading

1. Selected Topics in Inorganic Chemistry - Malik, Madan & Tuli.
2. Katakis, D. & Gordon, G. *Mechanism of Inorganic Reactions*, John Wiley & Sons: N.Y. (1987).

MCH-403: ORGANOMETALLIC CHEMISTRY-II

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-403	XX(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Fluxionality and Dynamic Equilibria 12 L

Stereo-chemical non-rigidity in organometallic complexes. Scrambling of carbonyl groups in metal carbonyl complexes. Fluxionality and dynamic equilibria in olefinic, π-allyl and cyclopentadienyl complexes. Ring whizzing. Davies-Green-Mingo (DMG) Rules.

Unit II: Distinctive Organometallic Reactions 12 L

Oxidative addition reactions (d^{10}, d^8 and d^7 complexes), Intramolecular oxidative addition reactions, C-H activation, cyclo-metallation and ortho-metallation, oxidative coupling reactions. Reductive elimination reactions (mono & binuclear systems), and β-elimination reactions, β-hydrogen elimination / β-hydrogen transfer reactions. Insertion reactions, insertion of carbonyls and alkene sand migratory insertion reactions.

Unit III: Compounds of Transition Metal-Carbon Multiple Bonds 14 L

Transition metal carbenes, Fischer carbene & Schrock's carbenes, their requisites and properties, Tebbe's reagent. Intermediate carbenes between Fischer & Schrock carbene, Grubb's catalyst 1st & 2nd generation catalyst and its applications. Transition metal carbyne complexes, their preparation properties and structures.

Unit IV: Industrial Applications of Organometallic Complexes 12 L

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 isomerization. Polymerization and Ziegler-Natta catalysis.

Essential Reading

1. Metallo-organic Chemistry – Anthony J. Pearson, John Wiley & Sons Inc. (1985).
2. Inorganic Chemistry – Principles of Structure & Reactivity, J. E. Huheey, Ellen A. Keiter & Richard L. Keiter, IV Edition (2005).
3. Introduction to Metal n-Complex Chemistry – M. Tsutsui, M.N. Levy, A. Nakamura, M. Ichikawa and K. Mori, Plenum Press, New York — Heme (1970).
4. Organometallic Chemistry – R. C. Mehrotra & A. Singh, Wiley Eastern Ltd. (2000).
5. Advanced Inorganic Chemistry – F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo & Manfred Bochmann, VI Edition, John Wiley & Sons Inc. (1999).

Suggested Reading

1. Infrared and Raman Spectra of Inorganic & Coordination Compounds; Kazuo Nakamoto, IV Edition, John Wiley & Sons Inc (1986).
2. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.

3. Comprehensive Coordination Chemistry Eds.: G. Wilkinson, R.D. Gillards and J.A. McCleverty, Pergamon

MCH-404: BIO-INORGANIC CHEMISTRY–II

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-404	XXI(i)	3	100 (UE=60, IA=40)	Inorganic Special

Unit I: Metallo-Proteins 12 L

Biological ligands for metal ions: Macrocycle, nucleobase, nucleotides and nucleic acids, coordination of metals by protein. Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, hemerythrin.

Unit II: Metallo-enzyme 12 L

Principle involved and role of various metals viz. Zn, Fe, Cu and Co; carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, zinc fingers, other gene regulatory zinc proteins, cobalamine, mutase activities of coenzyme B_{12}.

Unit III: Iron-Sulfur and other Non-Heme Proteins 14 L

Rubredoxine. Structure and function of iron sulphur proteins, cytochromes, cytochrome P-450, oxygen transfer, long distance electron transfer.

Unit IV: Application of Bioinorganic Chemistry 12 L

Medicinal and therapeutic; metal deficiency and disease, toxic effect of metals, metals used for diagnosis and chemotherapy, gold compounds as anti-rheumatic agents. Nitrogen cycle; biological nitrogen fixation, metalloenzyme in biological nitrogen cycle, molybdenum nitrogenase, other nitrogenase models.

Essential Reading

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

Suggested Reading

1. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J.J. Lippard, Wiley.
2. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983).

MCH-405: TECHNICAL CERAMICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-405	XVIII(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Piezoelectric and Optoelectric Ceramics 08 L

History of development, centrosymmetric and noncentrosymmetric (n.c.s.) crystals, polarization in n.c.s. crystals, piezoelectric ceramics, piezoelectric equations, definition of piezoelectric terms and their characteristics, poling of piezoelectric ceramics, dimensional changes. Ferroelectric ceramics: general features and applications. Electropic ceramics (e.o.c.): general aspects, birefringence in e.o.c., optical phase retardation, generation of various colours, electrotropic coefficients r and R, mode of application of e.o.c., characteristics required in e.o.c., composition systems: role of donors, acceptors and isovalent additives, processing and fabrication; loop in e.o.c. special features, intermediate polarization state, different types of hysteresis loop; electrochemical properties, piezoelectric deformation (extended treatment); applications.

Unit II: Ferrite Ceramics 12 L

Magnetic ferrites – general aspects, ferromagnetic, anti-ferromagnetic ordering in spinels, site preference in spinels, garnet, magnetic moments and occupancy of A&B sites, various ferrite compositions and their magnetic properties. Processing of ferrites – extended treatment. Non-microwave ferrite compositions, their B/H and other characteristics, applications; microwave ferrites – characteristics and applications.

Unit III: Ceramics Sensors 14 L

General aspects, intrinsic and extrinsic conductors, NTC thermistors – history of development; NTC device construction principle, device types and dimensions, electrical properties, resistivity-temperature behaviour, stability and sensitivity of thermal sensors, time constant and dissipation constant. Device chemistry – dependence of B and resistivity upon composition. Factors affecting sensor performance, stability and life resistance shift on aging, thermophysical properties of thermistor materials. NTC sensor applications, PTC thermistors – history of development, general applications, PTC thermistors – electrical behaviour, resistivity-temperature relationship, other electrical parameters, V-I curve – important features.

Device Chemistry – role of dopant, isovalent, altervalent and barrier layer modifiers, sintering aids, curie temperature control. **Gas Sensors** – general aspects, self-generating galvanic type oxygen sensors, construction, special features; modulating type gas sensors – general aspects, material requirements, temperature dependence of resistivity, its control.

Unit IV: Bioceramics 14 L

Bioceramics, bioinert versus biocompatible materials, partially stabilized zirconia, carbons and carbon-composite ceramics, mica glass ceramics, biocative ceramics – bioactive glass: bone bonding, conventional bioactive glasses, sol-gel routes to bioactive glass, problems of longevity of implant use, bioceramic composites, composites based on HAP, bone graft materials and applications.

Essential Reading

1. Introduction to Fine Ceramics by Noboru Ichinose (ed.), John Wiley and Sons, New York (1987).

2. Introduction to Fine Ceramics by Noburu Ichinose (ed.), John Wiley and Sons, New York (1987).

3. Ceramic Materials for Electronics – R.C. Buchanan (ed.), Marcel Deller, New York (1991).

4. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (eds.), Marcel Deller, New York.

5. Chemistry of Advanced Materials, an overview (ed.) by Leonard V. Interrante, Mark J. Hampden-Smith, John Wiley and Sons, New York, Marcel Deller, New York.

MCH-406: TECHNICAL CERAMICS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-406	XIX(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Preparation of Thin Films of Crystals 12 L

Electrochemical methods: anodic oxidation, cathodic deposition, electro-less deposition.
Chemical method: chemical vapour deposition, sol gel method, Langmuir Blodgett, photolithography
Physical methods: cathode sputtering, magnetron sputtering, vacuum evaporation, molecular beam epitaxy.
Application techniques: spin coating, flow coating, dip coating and printing (screen printing, gravure printing, flexo printing and ink jet printing)

Unit II: Preparation of Solid Solutions 10 L

General concepts on the requirement solid solution formation, substitution solid solutions, interstitial solid solution, Mechanism of complex solid solutions, Creation of cation, anion vacancies, creation of interstitial of cations and anions, double substitution, experimental techniques for studying solid solutions

Unit III: Characterization of Crystals Structures 12 L

X-ray techniques: X-ray diffraction and Bragg Law, Diffraction under ideal and non-ideal condition, X-ray scattering and structure factor, X-ray diffractometer, X-ray data file analysis,
Chemical analysis by emission (X-ray fluorescence), X-ray absorption techniques (AEFS, EXAFS)
Single crystal X-ray diffraction, different cameras and their special features
Electron spectroscopic techniques: principles, instrumentation, data analysis and applications of UPS, XPS, AES, Electron loss energy spectroscopy, neutron diffraction

Unit IV: Electron Microscopic and Thermal Characterization of Crystals Structures 14 L

Scanning Electron Microscopy – basic principle, instrumentation, electron specimen interaction, topographical and atomic number contrast, Transmission Electron Microscopy; practical aspect of microscopy, amplitude and phase contrast imaging, kinematical theory of image contrast, electron diffraction.
Atomic Force Microscopy: basic principles, Atomic Force Microscopy modes, phase imaging, face curve, application of Atomic Force Microscopy
Thermal techniques: principles, instrumentation, data analysis and applications of DSC, TGA, DTA and their special features

Essential Reading

1. Introduction to Materials Chemistry by H.R. Allcock Wiley.
2. Elements of X-Ray Diffraction (3rd Edition) by B. D. Cullity and S.R. Stock.
3. Introduction to X-Ray Powder Diffractometry by Ron Jenkins and Robert Snyder.

Suggested Reading

1. Understanding Solids: The Science of Materials by Richard Tilley (Wiley).
2. Scanning and Transmission Electron Microscopy: An Introduction by Stanley L. Flegler.
3. John W. Heckman Jr., and Karen L. Klomparens.

MCH-407: POLYMER TECHNOLOGY, PROCESSING AND SPECIALITY POLYMERS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-407	XX(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Polymer Technology – II 10 L

Additives for Plastics: Fillers, Plasticizers, Stabilizers, Lubricants, Flame Retardants, Foaming Agents, Crosslinking Agents,
Manufacture, Properties and Applications of Major Thermoplastics and Thermosetting Polymers: PE, PP, PVC, PS, Polyamides, Polyesters, Phenolic Resins, Amino Resins and Epoxy Resins, Polymeric Coatings

Unit II: Polymer Processing 10 L

Classification of Polymer Processing, Simple Model Flows for Analyzing Processing Operations with Examples,
Extrusion and Extruders, Calendering, Film Blowing, Injection Molding, Blow Molding, Rotational, Transfer and Compression Molding, Vacuum Forming, Reaction Injection Molding

Unit III: Biopolymers 14 L

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

Unit IV: Specialty Polymers 12 L

Conductive Polymers: Theory of Conduction, Synthesis and Applications of Conductive Polymers,
Biodegradable Polymers, Biomaterials, Polymers in Medicine, Drug Delivery Systems, Recycling of Polymers

Essential Reading

1. Text Book of Polymer Science By F. W. Billmeyer
2. Introduction to Polymers by R. J. Young and P. A. Lovel
3. Polymer Chemistry by G. Challa

Suggested Reading

1. Polymers: Chemistry and Physics of Modern Materials by JMG Cowie
2. Principles of Polymerization by George Odian

MCH-408: PROPERTIES OF MATERIALS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-408	XXI(ii)	3	100 (UE=60, IA=40)	Material Special

Unit I: Electronic State in Solids 12 L

Free electron theory of standing and running waves, density of state, band theory, K-space and Brillouin zones, band structures of metals, insulator and semiconductors,
the concept of hole, extrinsic (impurity) semiconductors, Fermi energy, position of Fermi level, free carrier concentration in intrinsic and extrinsic semiconductors,
application of semiconductors, application of semiconductors, I-VI compounds, I -IV compounds, III-V compounds

Unit II: Electrical Properties 14 L

Introduction, electron drift in an electrical field, relaxation time and mean free path, electrical conductivity of non-degenerate and degenerate gases,
specific conductance of conductor, Wiedemann-Franz-Lorentz law, electrical conductivity of metals and alloys,
piezoelectric materials temperature dependence, carrier mobility, electrical conductivity of pure metal, electrical conductivity of alloys.

Unit III: Magnetic Properties 10 L

Introduction: Classification of magnetic materials, diamagnetism, paramagnetic, ferromagnetic anisotropy,
ferromagnetic domains, origin of domain wall antiferromagnetism, antiferromagnetic domains, ferrimagnetism,
normal spinel's inverse spinels, ferromagnetic domain.

Unit IV: Optical Properties 10 L

Introduction: Refractive index, dispersion, absorption, birefringence, photoluminescence laser, nonlinear optical materials — non-linear optical effect,
second and third order molecular hyperpolarisability and second order electric susceptibility materials for second and third order harmonic generation.

Essential Reading

1. Solid State Physics by Epifanov.
2. Materials Science by Anderson and Lever.

MCH-409: MEDICINAL CHEMISTRY AND BIOMOLECULES

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-409	XVIII(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Drug Design 8 L

Concept of lead compound, lead modification, prodrugs and soft drugs, structure–activity relationship (SAR), factors affecting bioactivity: resonance, inductive effect, isosterism, bioisosterism, spatial considerations. Occupancy theory, rate theory, induced fit theory. Concepts of drug receptors. Free–Wilson analysis, Hansch analysis, relationship between Free–Wilson and Hansch analysis. LD_{50}, ED_{50} (mathematical derivations of equations excluded).

Unit II: Mechanism of Drug Action and Chemotherapeutics 12 L

Mechanism of drug action: enzyme stimulation and inhibition, types of inhibition, antimetabolites (sulphonamides and their classification). Synthesis of Penicillin G, Ampicillin, Tetracycline, Ciprofloxacin. Drug metabolism: metabolic and conjugation reactions. Cardiovascular diseases: synthesis of amyl nitrate, sorbitrate, diltiazem and oxyprenolol. Drug chemotherapeutics and pharmacodynamic agents.

Unit III: Nucleic Acids 14 L

Introduction, structures and functions of DNA and RNAs (m-RNA, t-RNA, r-RNA). Chemical and enzymatic hydrolysis of DNA and RNAs. Overview of gene expression: replication, transcription and translation. Genetic code: origin and Wobble hypothesis. Genetic errors, mutation and carcinogenesis, recombinant DNA technology. Molecular recognition of DNA. Recognition and modulation of DNA, RNA, and proteins with small molecules.

Unit IV: Protein Chemistry 8 L

Introduction. Structure of peptides and proteins: primary, secondary and tertiary structures; non-covalent interactions and aggregation. Protein folding and factors affecting it. Degradation of amino acids, urea cycle, uric acid and ammonia formation.

Books Suggested

- A. Gringauge, *Introduction to Medicinal Chemistry*, Wiley-VCH.
- J. D. Watson, *Molecular Biology*, The Benjamin/Cumming Company, Inc.
- R. B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, Academic Press.
- D. Lednicer, *Strategies for Organic Drug Synthesis and Design*, John Wiley & Sons Ltd.
- Surendra N. Pandeya, *A Text Book of Medicinal Chemistry*, Vol-I and Vol-II, S. G. Publishers.
- Ashutosh Kar, *Medicinal Chemistry*, New Age International Publishers.
- *Goodman and Gilman's Pharmacological Basis of Therapeutics*, McGraw-Hill.
- M. E. Wolff (Ed.), *Burger's Medicinal Chemistry and Drug Discovery*, Vol. I–V, John Wiley & Sons Ltd.
- L. Stryer, *Biochemistry*, 4th Ed., W. H. Freeman & Co., USA.

MCH-410: MEDICINAL CHEMISTRY AND BIOMOLECULES

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-410	XIX(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Carbenes, Carbenoids and N-Heterocyclic Carbenes (NHC) 12 L

Introduction, Fischer and Schrock carbenes with their synthetic applications. Dotz benzannulation reaction. The nature of N-heterocyclic carbenes: Synthesis (synthesis of the imidazolium salts and transition metal complexes of NHC) and properties (basicity of NHC, steric properties, and decomposition pathways of NHC).
Reactions based on carbenes insertions into C–H, N–H, and O–H bonds. Ring closing metathesis (RCM), ring opening metathesis (ROM), enzyme metathesis (EM), ring-closing-ring-opening metathesis (RCM-ROM), cross metathesis (CM) and tandem metathesis.

Unit II: Radical Chemistry 12 L

Introduction, generation of radicals, addition to a pi-bond, fragmentation, atom abstraction (reaction with a sigma bond), radical-radical combination, disproportionation, electron transfer, addition of a nucleophile, and loss of a leaving group.
Minisci reaction, Kagan-Molander coupling, Sandmeyer reaction, and Hunsdiecker reactions.

Unit III: C-H Bond Functionalization/Activation 08 L

Definition and challenges & logic of C–H functionalization, alpha C–H functionalization of ethers and alcohols, diastereo control in C–H methylene group, sp^2 C–H functionalization, activated sp^3 C–H functionalization (allyl, benzyl, propargyl and carbonyl); alpha heteroatomic hydrogen), oxidative C–H functionalization, metalloporphyrin complex in C–H functionalization and other new particularly in the development of novel catalytic methodologies for multiple C–H (sp^2, sp^3) functionalization.

Unit IV: Multicomponent Reactions (MCRs) 14 L

History of multicomponent chemistry, the discovery of new isocyanide-based multicomponent reactions, multicomponent reactions with carbonyl compounds, metal-catalyzed multicomponent reactions and their applications:
Hantzsch synthesis of dihydropyridines, Strecker synthesis of α-amino acids, The Biginelli reaction, Bucherer-Bergs reaction, Passerini reaction, Ugi reaction, and the Domino-Knoevenagel-Hetero-Diels-Alder reaction.

Essential Reading:

1. Kurti, L. and Czako, B. *Strategic Applications of Named Reactions in Organic Synthesis* (2004).
2. Carruthers, W. and Coldham, I. *Modern Methods of Organic Synthesis*, Cambridge University Press (2004).
3. D'Souza D. M., Müller T. J. J. *Multi-component Syntheses of Heterocycles by Transition-Metal Catalysis*. Chem. Soc. Rev. 2007, 36:1095–1120.
4. *Organometallic Reagents in Synthesis* by Paul R. Jenkins.
5. *N-Heterocyclic Carbenes in Transition Metal Catalysis* by Frank Glorius, Springer-Verlag, Berlin Heidelberg 2007.

Suggested Reading:

1. *Organometallic Chemistry*, R. C. Malhotra & A. Singh, Wiley Eastern Ltd. (2000).
2. Bruckner, R. *Advanced Organic Chemistry*, Elsevier (2002).
3. Clayden, Greeves, Warren & Wothers, *Organic Chemistry*, Oxford University Press (2001).
4. A. L. Lehninger, *Principles of Biochemistry*, W. H. Freeman & Co., USA.

MCH-411: CHEMISTRY OF NATURAL PRODUCTS

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-411	XX(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: Terpenoids 12 L

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, synthesis of the following representative molecules: Citral, geraniol, α-Pinene, Camphor

Unit II: Alkaloids 12 L

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Morphine.

Unit III: Steroids 8 L

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Androsterone, Testosterone, Estrone, Progesterone.

Unit IV: Prostaglandins and Flavonoids 14 L

Discuss about the structure Prostaglandins and Flavonoids. Occurrence, nomenclature and general methods of structure determinations, isolation and synthesis, Quercetin, Flavones, Flavonols.

Essential Reading:

1. I.L. Finar, Organic Chemistry, Vol. II, ELBS Publications, UK.
2. J. Mann, R.S. Devison, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, *Natural Products Chemistry and Biological Significance*, Longman Publisher, Essex, UK.
3. B.A. Bohm, *Introduction to Flavonoids*, Harwood Academic Publishers, USA.
4. *Natural Products – Chemistry and Biological Significance*, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
5. *Organic Chemistry Vol. II*, I.L. Finar, ELBS. *Stereo Selective Synthesis – A Practical Approach*, M. Nogradi, VCH.

Suggested Reading:

1. *Rodd's Chemistry of Carbon Compounds*, Ed. S. Coffey, Elsevier.
2. *Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas*, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
3. *Introduction to Flavonoids*, B. A. Bohm, Harwood Academic Publishers.
4. *New Trends in Natural Product Chemistry*, Atta-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.

5. *Insecticides of Natural Origin*, Sukh Dev, Harwood Academic Publishers.

MCH-412: APPLICATIONS OF SPECTROSCOPY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-412	XXI(iii)	3	100 (UE=60, IA=40)	Organic Special

Unit I: UV-visible and IR Spectroscopy 12 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: Applications of ^{1}H and ^{13}C NMR Spectroscopy 12 L

First-order and Non-first-order spectra, spin-spin interaction between two, three, four and five nuclei (first order spectra), factors affecting coupling constant "J", classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Resolution and multiplicity of ^{13}C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; un-decoupled, Proton decoupled, Off resonance, factors affecting chemical shifts. Structural applications of ^{1}H and ^{13}C-NMR.

Unit III: 2D NMR Techniques 8 L

General idea about two dimensional NMR spectroscopy, APT, INEPT, DEPT, Correlation spectroscopy (COSY) - Homo COSY (1H-1H), TOCSY, Hetero COSY (HMSC, HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Unit IV: Optical Rotatory Dispersion and Circular Dichroism 14 L

Cotton effect, types of ORD and CD curves – similarities and difference between ORD and CD curves and their application to stereochemical problems; Octant rule and its application in structural studies, lactone sector and α-Halo keto rule.

Essential Reading:

1. Kemp, W. Organic Spectroscopy, W.H. Freeman & Co.
2. R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectroscopic Identification of Organic Compounds, John Wiley & Sons.
3. M. L. Martin, J. J. Delpeuch and G. J. Martin, Heyden, Practical NMR Spectroscopy, Spectrometric Identification of Organic Compounds, John Wiley.
4. R. J. Abraham, J. Fisher and P. Loftus, Introduction to NMR Spectroscopy, Wiley.
5. J. R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall.
6. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill.
7. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for RD and CD and ESR.

MCH-413: ADVANCED MOLECULAR SPECTROSCOPY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-413	XVIII(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Introduction to Molecular Spectroscopy 15 L

Time dependent perturbation. Einstein coefficients, Lambert–Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.
Electronic Spectroscopy: Electronic spectroscopy of organic molecules – benzene, effect of substitution – pyridine, pyrimidine, pyrazine, methyl substitution. Vibronic analysis.

Unit II: Vibrational Spectroscopy 11 L

Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules: BF_3, NH_3. Square planar, trigonal bipyramidal, framework and cage molecules. Jahn–Teller distortions.

Unit III: Magnetic Resonance Spectroscopy 10 L

Electronic Spin Resonance spectroscopy. Basic principles. Relaxation and Line Widths. Zero-field splitting and Kramer's degeneracy. Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra. Applications of ESR spectroscopy: Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and o-, m- and p- xylene radical ions from HMO theory. Study of unstable paramagnetic species, Kinetic studies of electron transfer reactions.
NMR Spectroscopy: Mechanism of spin-spin spin-lattice relaxations and quantitative treatment of relaxations. Quantum mechanical treatment of the AB system. Selection rules and relative intensity of lines.

Unit IV: Mossbauer and other Spectroscopic Methods 09 L

Principles of Mossbauer spectroscopy: Isomer shifts. Quadrupole and nuclear Zeeman splitting. Applications in structure determination.
Photoelectron Spectroscopy: Basic principles of PES/ESCA and Auger spectroscopy to the study of surfaces.

Essential Reading:

1. D. C. Harris & 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, U.K. (1973).
3. A. Carrington & A.D. Maclachlan. *Introduction to Magnetic Resonance*, Chapman & Hall, NY (1983).
4. J.E. Wertz & J.R. Bolton. *Electron Spin Resonance, Elementary Theory and Practical Applications*, Chapman & Hall, NY (1986).
5. S. R. Chang, *Basic Principles of Spectroscopy*, McGraw-Hill, 1971.
6. R.V. Parish, *NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry*, Ellis Horwood Series, 1990.

7. C.L. Briant & R.P. Messmer, *Auger Electron Spectroscopy*, Treatise on Materials Science and Technology, Vol. 30, Academic Press Inc., 1988.

MCH-414: NANO CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-414	XIX(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Fundamentals of Nanoscience and Technology 07L

Perspective of length. Nanomaterials and chemistry of advanced materials and nanostructures. Solid materials and their strength, surface effects, prime materials. Carbon nanostructures: Graphene, Fullerenes, and Carbon Nanotubes (SWCNT and MWCNT). Surface plasmon resonance and quantum size effects.

Unit II: Applications of Nanomaterials 06L

(a) General Applications: Nanomaterials based on gold, silver, dielectric/magnetic oxides. Applications in health and medicines, environment and water purification, automobiles, sensors, batteries, computers, communication, food, paint, textile and ceramics industry.
(b) Functional Applications: Nanocatalysis, photocatalysis, electrocatalysis, photoelectrocatalysis, water splitting, and green/renewable energy.

Unit III: Synthesis of Nanomaterials 12L

Overview of synthesis routes: solvothermal, hydrothermal, reverse micellar/microemulsion, sol-gel, polymeric citrate precursor, co-precipitation and sonochemical methods. Theory, experimental conditions, and kinetics of solid-state reactions and molten-salt routes.

Unit IV: Characterization of Nanomaterials 15L

(a) Structural elucidation using X-ray diffraction: Laue and powder methods, particle size determination using X-ray line broadening (Scherrer's formula).
(b) Theory, instrumentation, and applications of SEM, TEM, AFM, and STM microscopies.
(c) Principle, theory, and methodology of Dynamic Light Scattering (DLS) and BET surface area studies.

Essential Reading

1. M. A. Shah and Tokeer Ahmad, *Principals of Nanoscience and Nanotechnology*, Narosa Publications, 2010.

2. B. Viswanathan, *Nano Materials*, Narosa Publications, 2009.

3. Nano: The Essentials, T. Pradeep, Tata McGraw Hill, 2009.

4. Chemistry of Nanomaterials: Synthesis, Properties and Applications by C.N.R. Rao, A. Muller and A. K. Cheetham (eds.), Wiley-VCH, Weinheim, 2004.

5. Nanoscale Materials by Luis M. Liz-Marzan and Prashant V. Kamat, Kluwer Academic Publishers (Boston), 2003.

6. *Nanomaterials Chemistry: Recent Developments and New Directions*, ed. by C.N.R. Rao, A. Muller & A.K. Cheetham (Eds.), Wiley-VCH, 2007.

Suggested Reading

1. M. A. Shah and Tokeer Ahmad, *Nano Science & Technology*, I.K. International Pvt. Ltd., 2021.

2. M. A. Shah and Tokeer Ahmad, *Principles of Nanoscience and Nanotechnology*, Narosa Publications, 2010.

3. T. Pradeep, *Nano: The Essentials*, Tata McGraw-Hill, 2009.

4. Luis M. Liz-Marzan and Prashant V. Kamat, *Nanoscale Materials*, Kluwer Academic Publishers, 2003.

5. C. N. R. Rao, A. Müller, and A. K. Cheetham (Eds.), *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH, 2007.

6. R. F. Egerton, *Physical Principles of Electron Microscopy: An Introduction to TEM, SEM and AFM*, Springer, 2008.

7. Paul E. West, *Introduction to Atomic Force Microscopy*, Pacific Nanotechnology.

MCH-415: ADVANCED PHYSICAL CHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-415	XX(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Molecular Structure in Biological Systems 15L

Forces stabilizing biomolecular conformation: hydrogen bonding, electrostatics, van der Waals, hydrophobic effects, and stereoelectronic interactions. Properties of water relevant to biological systems: polarity, dielectric constant, hydrogen bonding. Thermodynamic principles in biomolecular stability: entropy, enthalpy, and free energy. Overview of amino acids: classification, zwitterionic nature, and protein structural hierarchy. Nucleic acids: nucleosides, nucleotides, DNA/RNA structures and base pairing.

Unit II: Conformational Analysis 12L

Polypeptide geometries, torsion angles, Ramachandran plots. Basics of molecular mechanics and stabilizing interactions in biomolecules. Challenges in macromolecular modeling. Energy minimization and structure refinement. Introduction to molecular dynamics simulations.

Unit III: Biopolymer Interactions and Non-equilibrium Thermodynamics in Biology 10L

Non-covalent interactions: electrostatic (dipole–dipole), dispersion forces, and hydrophobic effects. Multiple equilibria and binding processes in biological systems. Thermodynamics of biopolymer solutions: Flory–Huggins theory of macromolecular solvation, osmotic pressure, and Donnan membrane equilibrium.

Unit IV: Statistical Mechanics and Biomolecular Simulations 15L

Chain configurations of macromolecules: random walk model and statistical distribution of end-to-end distances; average dimensions of various polymer chain structures. Conformational transitions: helix–coil transition and the protein folding problem. Molecular mechanics and dynamics: basic principles, molecular representations, force fields, atom–atom pair potentials, bond length, bond angle, torsional potentials, van der Waals and electrostatic interactions. Introduction to time-step integration algorithms and simulation force fields.

Essential Reading

1. C. R. Cantor & P. R. Schimmel, *Biophysical Chemistry*, Vols. 1–3, W. H. Freeman (1980).
2. Michel Daune, *Molecular Biophysics: Structures and Dynamics*, Oxford University Press.
3. Thomas E. Creighton, *The Biophysical Chemistry of Nucleic Acids & Proteins*, Helvetica Press.
4. M. V. Volkenstein, *Molecular Biophysics*, Academic Press.
5. Y. Moroi, *Micelle: Theoretical and Applied Aspects*, Plenum Press, New York, 1992.
6. A. J. Bard & L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., Wiley (2002).
7. D. Frenkel & B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press.

8. M. P. Allen & D. J. Tildesley, *Computer Simulation of Liquids*, Oxford University Press.

9. T. E. Creighton, *The Physical and Chemical Basis of Molecular Biology*, Helvetica Press.

MCH-416: ELECTROCHEMISTRY

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-415	XXI(iv)	3	100 (UE=60, IA=40)	Physical Special

Unit I: Electrolyte Solution 12 L

Structure of water, effect of an ion on the structure of water, solvation number, activity, activity coefficients and ion–ion interactions, physical significance of activity coefficient of an electrolyte. Determination of mean ionic activity coefficient by freezing point depression and EMF measurement methods. Limiting law, electrochemical potential. Derivation of Debye–Hückel–Onsager equation.

Unit II: Electrode Kinetics 10 L

Charge transfer under zero field and under the influence of an electric field. Two-way electron transfer, equilibrium exchange current density, interface out of equilibrium. Derivation of Butler–Volmer equation, Tafel plots, multistep reactions.

Unit III: Transport Phenomena 11 L

Diffusion coefficients. Fick's first and second laws (steady and non-steady state diffusion), relation between diffusion coefficient and mean free path. Relation between thermal conductivity/viscosity and mean free path of a perfect gas. Einstein's relation between diffusion coefficient and absolute ionic mobility. Stokes–Einstein equation, Nernst–Einstein equation, Nernst–Planck flux equation.

Unit IV: Adsorption and Electrical Double Layer 12 L

Electrical double layer and thermodynamics of electrified interfaces. Derivation of electrocapillary equation, determination of charge density on electrodes, electrical capacitance of the interface. Models of the electrical double layer: Helmholtz–Perrin, Gouy–Chapman, Stern, Graham–Devanathan–Mott-Watts, Tobin, Bockris–Devanathan models.

Suggested Reading

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

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

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

MCH-417: CHEMISTRY OF SYNTHETIC AND NATURAL MATERIALS-II

Semester	Paper Code	Paper No.	Credits	Total Marks	Paper Type
IV	MCH-417	XXII	4	100 (UE=60, IA=40)	Theory (Elective)

Unit I: Applications of High Tc Materials 15L

Applications of High Tc Superconductors; Superconductivity applications in power systems; high and low temperature superconductors and their preparation; Properties of High Tc materials: anisotropy, penetration depth; SQUID magnetometers; Superconducting IR detectors; Superconductor-based microwave devices; Josephson junctions; Application of superconductors in imaging and diagnostics.

Unit II: Supramolecular Chemistry 12L

Introduction, host–guest interactions, classification of host–guest compounds, intermolecular forces, nature of supramolecular interactions, molecular recognition, chiral discrimination, molecular receptors and design principles, template effect, cryptands, cyclodextrins, calixarenes, calix pyrroles, crown ethers, catenanes, rotaxanes, molecular capsules, and molecular self-assembly.

Unit III: Advanced Quantum Mechanics 10L

Review of quantum mechanics; Born–Oppenheimer approximation; Slater codon rules; Hartree–Fock equation; Koopman and Brillouin theories; Roothaan equation; Gaussian basis sets.

Unit IV: Excited States of Metal Complexes 15L

Concept of excited states in metal complexes; Comparison with organic compounds; Electronically excited states; Charge transfer spectra; Charge transfer excitations; Methods for obtaining charge transfer spectra; Metal complex sensitizers; Electron relay; Metal colloid systems.

Essential Reading

1. J. M. Lehn, *Supramolecular Chemistry*, Wiley-VCH.
2. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley, 2002.
3. H.-J. Schneider and A. Yatsimirsky, *Principles and Methods in Supramolecular Chemistry*, John Wiley, 2000.
4. *Chemical Safety Matters*, IUPAC–IPCS, Cambridge University Press, 1992.
5. *OSU Safety Manual* 1.01.

Suggested Reading

3. Waldman & Janning, *Chemical Biology: A Practical Course*, Wiley-VCH, 2004.
4. Joseph R. Lakowicz, *Principles of Fluorescence Spectroscopy*, Springer, 2006.