Madhabdev University

(A State University Established under the Assam Act. No. XXXV of 2017)

Curriculum and Syllabus

Of

Two Year Postgraduate Programme

In

Chemistry

From Academic Session

2026-2027

Department of Chemistry
Narayanpur, P.O.: Dikrong (784164), Dist.: Lakhimpur, Assam

Course Distribution

Sem	Paper	Paper Name	Paper Code	Marks Distribution		Credit Distribution		Total credit
				In-Sem	End-Sem	Theory	Practical/ Tutorial	
I	*Major I*	*Advanced Inorganic Chemistry- I*	CHMP-101	30	70	4	0	4
	Major II	*Advanced Organic Chemistry -I*	CHMP-102	30	70	4	0	4
	Major III	*Advanced Physical Chemistry -I*	CHMP-103	30	70	4	0	4
	Major IV	*Research Methodology for Natural Sciences*	CHMP-104	30	70	3	1	4
	Major V	*Advanced Practical Chemistry I/ Research Project*	CHMP-105	30	70	0	2	2
	Minor VII	*General Chemistry IX*	CHMN-701			4	0	4
					Total	20	2	22
II	*Major V*	*Advanced Inorganic Chemistry- II*	CHMP-201	30	70	4	0	4
	Major VI	*Advanced Organic Chemistry –II*	CHMP-202	30	70	4	0	4
	Major VII	*Advanced Physical Chemistry -II*	CHMP-203	30	70	4	0	4
	Major VIII	*Advanced Practical Chemistry II*	CHMP-204	30	70	0	4	4
	Major IX	*Advanced Practical Chemistry II/ Field Work/*	CHMP-104	60	140	0	4	4
	Minor VIII	*General Chemistry IX*	CHMN-801			4	0	4
					Total	16	4	24
III	*Major IX*	*Advanced Inorganic Chemistry- III*	CHMP-301	30	70	4	0	4
	Major X	*Advanced Organic Chemistry -III*	CHMP-302	30	70	4	0	4
	Major XI	*Advanced Physical Chemistry -III*	CHMP-303			4	0	4
	Major XII	*Elective Course*	CHME-30X			4	0	4
	Major XIII	*Advanced Practical / Research Project*	CHMP-304			0	4	4
					Total	16	4	20
II	*Major I*	*Advanced Inorganic Chemistry- IV*	CHMP-401	30	70	4	0	4
	Major II	*Advanced Organic Chemistry-IV*	CHMP-402	30	70	4	0	4
	Major III	*Advanced Physical Chemistry -IV*	CHMP-403			4	0	4
	Elective	*Elective Course*	CHME-40X			4	0	4
		Research Project/Advanced practical and literature survey				0	4	4
					Total			20

Elective Courses

PG Semester III (any one from the following group)	
Paper Code	*Paper Name*
CHME-301	*Elective-I (Advanced Solid State Chemistry and Functional Materials)*
CHME-302	*Elective – III (Advanced Polymer Chemistry)*
CHME-303	*Elective-III (Molecular Rearrangements and Reactive Intermediates in Organic Synthesis)/MOOCS*
CHME-304	*Elective – IV (Transition Metal Organometallic Chemistry: Principles to Applications)/MOOCS*
CHME-305	*Elective-V (Advanced Stereochemistry and Organic Reactions)*
PG Semester IV (any one from the following group)	
CHME-401	*Elective VI (Advanced Catalysis and Catalytic Materials)*
CHME-403	*Elective VII (Advanced Environmental Chemistry)*
CHME-403	*Elective VIII (Nanoscience and Nanomaterials)*
CHME-404	*Elective IX (Classics in Total Synthesis)*

PG Semester I

NCrF level	*6.0*
Title of the Course	*Advanced Inorganic Chemistry - I*
Course code	*CHMP-101*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop an advanced understanding of the mechanisms of substitution, isomerization, and electron transfer reactions in coordination compounds and correlate reaction pathways with kinetic and stereochemical evidence.
- Explain advanced bonding theories of coordination compounds, including Ligand Field Theory (LFT) and Molecular Orbital Theory (MOT), and interpret their electronic spectra using Tanabe–Sugano diagrams, Racah parameters, and nephelauxetic effects.
- Acquire comprehensive knowledge of organometallic chemistry involving metal carbonyls, carbenes, metallocenes, metal arene complexes, and homogeneous catalysis, with emphasis on their synthesis, bonding, structure, reactivity, and applications.
- Understand the crystal structures, bonding, and properties of important inorganic solids and relate lattice energy to their physical and chemical behaviour.
- Explain the structure, function, and catalytic roles of biologically important metal-containing enzymes and metalloproteins involved in essential biological processes.
- Develop analytical, problem-solving, and scientific reasoning skills for interpreting reaction mechanisms, spectroscopic data, structural features, and contemporary applications of inorganic chemistry.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the mechanisms of substitution, hydrolysis, aquation, anation, isomerization, racemization, and electron transfer reactions in coordination complexes using kinetic and stereochemical evidence.

CO2: Apply Ligand Field Theory and Molecular Orbital Theory to explain bonding, magnetic properties, electronic spectra, Racah parameters, nephelauxetic effect, charge transfer transitions, and crystal field stabilization energies of coordination compounds.

CO3: Explain the synthesis, bonding, structure, reactivity, fluxional behaviour, and catalytic applications of organometallic compounds, including metal carbonyls, metal carbenes, metallocenes, and metal arene complexes.

CO4: Interpret spectroscopic evidence (UV–Visible, EPR, and multinuclear NMR) for elucidating the structure and dynamics of inorganic and organometallic compounds.

CO5: Describe the crystal structures, lattice energies, and structure–property relationships of important inorganic solids.

CO6: Explain the structure and biological functions of metalloproteins and metalloenzymes involved in photosynthesis, nitrogen fixation, oxidation, reduction, and coenzyme-mediated biochemical reactions.

Unit I Reaction Mechanism in Coordination chemistry- II — *Lecture/Marks: 20*

Substitution reactions in octahedral complexes, Evidences for dissociative mechanism, water exchange, anation, aquation or hydrolysis (details of rate equation), factors affecting in acid hydrolysis, stereochemistry of acid catalysed reaction, isomerization and racemization of octahedral complexes, substitution reaction without braking metal-ligand bond

Substitution reaction in square planner complexes, factors affecting rates of substitution reaction, mechanism of substitution reaction of square planner complexes, evidences in favour of associative mechanism, application of trans effect

Electron transfer reaction, outer-sphere and inner-sphere mechanism, salient features of these mechanism, Cross reaction, Marcus theorem, acceleration of rate of electron transfer reaction, inner-sphere reaction of complex with organic ligand, successor complex and fission, redox reaction with two electron involvement, complementary and non-complementary reaction, use of electron transfer reactions for synthesising complexes

Unit II Bonding theories and Electronic spectra of coordination Complex — *Lecture/Marks: 15*

Demerits of CFT, nephelauxetic effect and EPR evidences, Racah parameters, Ligand field theory, Molecular orbital theory, charge transfer spectra, Tanabe sugano diagram, and calculation of B and CFSE

Unit III Organometallic chemistry II: Carbene and catalysis — *Lecture/Marks: 15*

Metal carbonylate ions: synthesis, properties and reactions
Metal carbonyl hydrides: synthesis, properties, bonding modes and spectral properties M-H bond
Metal carbonyl halides: synthesis and reactions
Fluxionality in organometallic compounds and spectral evidences (^{1}H, ^{13}C, ^{31}P NMR)

Metal carbenes: Introduction to metal-carbon multiple bonds, classifications, Fischer carbene, Schrock carbene, (Synthesis, Structure, bonding, synthesis and application), Tebb's reagent metal carbynes

Bonding in cyclobutadiene, cyclopentadiene
Ferrocene: Preparation and reactions (acetylation, alkylation, nitration and halogenation, metallation, Mannich condensation). Structure and aromaticity, Comparison of aromaticity and reactivity with that of benzene, other metallocences
Metal arene complexes: Synthesis, properties, reactions

Unit IV Inorganic solid — *Lecture/Marks: 10*

Characteristic structure types of ionic solids: CsCl, NaCl, Spalerite and Wurtzite types of ZnS, fluorite and anti-fluorite, nickel arsenide, $CdCl_2$, CdI_2, rutile, perovskite and spinels, Lattice enthalpy, consequences of lattice enthalpy

Unit V Bioinorganic Chemistry IV — *Lecture/Marks: 10*

Photosynthesis: reaction pathway, role of magnesium ions
Active site structure and activity of nitrogenase enzyme, xanthine oxidase, alcohol dehydrogenage, aldehyde oxidase, aldehyde dehydrogenase and V-B_{12}

Suggested reading

- F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, Wiley.
- J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson.
- Miessler, Fischer & Tarr, *Inorganic Chemistry*, 5th Edition, Pearson.
- Gary L. Miessler, Paul J. Fischer & Donald A. Tarr, *Inorganic Chemistry*, Pearson.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J. & Armstrong, F., *Inorganic Chemistry*, Oxford University Press.
- Satya Prakash, G. D. Tuli, S. K. Basu & R. D. Madan, *Advanced Inorganic Chemistry*, S. Chand.
- P. L. Soni & Mohan Katyal, *Textbook of Inorganic Chemistry*, Sultan Chand & Sons.
- R. P. Sarkar, *Inorganic Chemistry*, Part I & II, NCBA
- Gurdeep Raj, *Advanced Inorganic Chemistry*, Goel Publishing House.
- B. R. Puri, L. R. Sharma & K. C. Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing Co.

PG Semester I

NCrF level	*6.0*
Title of the Course	*Advanced Organic Chemistry - I*
Course code	*CHMP-102*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop an advanced understanding of selective oxidation and reduction reactions, their mechanisms, reagent chemistry, stereochemical aspects, and synthetic applications in organic chemistry.
- Explain the mechanisms of important molecular rearrangements involving carbon, oxygen, nitrogen, and aromatic systems, and predict the products based on mechanistic pathways.
- Acquire comprehensive knowledge of the synthesis, properties, reactions, stereochemistry, and analytical aspects of amino acids, peptides, and nucleic acids.
- Apply mechanistic concepts to design efficient synthetic routes using appropriate oxidizing agents, reducing agents, and rearrangement reactions.
- Correlate reaction mechanisms with regioselectivity, chemoselectivity, stereoselectivity, and reaction conditions in modern organic synthesis.
- Develop problem-solving skills for interpreting reaction mechanisms, retrosynthetic analysis, and biomolecular transformations relevant to research, pharmaceutical chemistry, and chemical industries.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the mechanisms, selectivity, and applications of important oxidation reactions using transition metal-, DMSO-, selenium-, and peroxide-based oxidizing reagents.

CO2: Select suitable oxidizing or reducing reagents for the chemoselective transformation of functional groups and predict reaction products under different conditions.

CO3: Describe the mechanisms and synthetic applications of catalytic hydrogenation, dissolving metal reductions, hydride reductions, borane reductions, and other important reduction reactions.

CO4: Analyze the mechanisms of molecular rearrangements involving carbon-, oxygen-, nitrogen-, and aromatic-centered migrations and apply them in synthetic organic chemistry.

CO5: Explain the synthesis, stereochemistry, properties, and reactions of amino acids and peptides, including modern peptide synthesis and sequence determination techniques.

CO6: Describe the structure, chemistry, hydrolysis, and biological significance of nucleic acids and explain the molecular basis of DNA structure and complementary base pairing.

CO7: Interpret reaction mechanisms, stereochemical outcomes, and synthetic strategies to solve advanced problems in organic synthesis.

Unit I: Oxidations ***Lecture/Marks: 15***

Oxidation of alcohols to aldehydes/ketones/carboxylic acids: Transition metal-based oxidants: Jones reagent, Collins Reagent, PCC, PDC, KMnO4, MnO2, Mn(OAc)3, RuCl3/NaIO4 (RuO4). Dimethyl sulfoxide-based oxidation: Moffatt-Pfitzner Oxidation, Parikh-Doering Oxidation, Corey-Kim Oxidation, Swern Oxidation. (B) Oxidation of alkenes/alkynes: Ozonolysis, KMnO4, Prévost dihydroxylation, Woodward dihydroxylation, epoxidation by peroxy acids and related reagents (C) Other oxidation processes: Allylic oxidation by SeO2, Oxidation of aldehydes/ketones by SeO2, Cleavage of 1,2-diols, Hunsdiecker reaction.

Unit II: Reductions ***Lecture/Marks: 15***

(A) Hydrogenation: H2/Pd-C, H2/Lindlar Catalyst, H2/Wilkinson's Catalyst, transfer hydrogenation, diimide reduction. (B) Dissolving Metal Reductions for: alkynes, aldehydes/ketones, esters, α,β-unsaturated ketones, aromatic compounds (Birch reduction), Clemmensen Reduction. (C) Aluminium-based reagents: lithium aluminum hydride (LAH), lithium trimethoxyaluminium hydride (LTBA), lithium tri-(tert-butoxy)aluminium hydride (LTBA), sodium bis(2-methoxyethoxy)aluminium hydride (Red-Al), selectrides, diisobutylaluminium hydride, alane. Boron-based reagents: Sodium borohydride, Zinc borohydride, Lithium borohydride, Sodium cyanoborohydride, Sodium triacetoxyborohydride, borane. (D) Other reduction processes: Wolff-Kishner reduction, Clemmensen Reduction, MPV reduction.

Unit III: Rearrangements ***Lecture/Marks: 20***

Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol pinacolon and related rearrangements, dienone-phenol rearrangement, benzil-benzilic acid rearrangement.

Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, hydroperoxide rearrangement cumene hydroperoxide-phenol rearrangement, Dakin reaction.

Rearrangement to electron-deficient nitrogen (Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement).

Aromatic rearrangements: Migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement), migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement, Benzidine rearrangement

Unit-IV: Amino acids ***Lecture/Marks: 20***

Amino acids: Synthesis with mechanistic details: Strecker, Gabriel; acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperizine, isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.

Peptides: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using N-protection & C-protection, solid-phase (Merrifield) synthesis; peptide sequence: C-terminal and N-terminal unit determination (Edman, Sanger and 'dansyl' methods); partial hydrolysis; specific cleavage of peptides; use of CNBr.

Nucleic acids: pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalyzed hydrolysis of nucleosides (both pyrimidine and purine types); comparison of alkaline hydrolysis of DNA and RNA; elementary idea of double helical structure of DNA (Watson-Crick model); complimentary base–pairing in DNA.

Suggested reading

- *Smith, M. B.; March, J., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley India, New Delhi (2015).*
- *Smith, M. B., Organic Synthesis, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).*
- *Greeves, N.; Clayden, J.; Warren, S., Organic Chemistry, 2nd Ed., Oxford University Press, New Delhi (2012).*
- Carruthers, W., Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, New Delhi (2005).
- Zweifel, G. S.; Nantz, M. H.; Somfai, P., Modern Organic Synthesis: An Introduction, 2nd Ed., Wiley-Blackwell, New York (2017)
- *D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry; 5th edition, 2008 (W. H. Freeman &Co.).*
- *R. H. Abeles, P. A. Frey, W. P. Jencks, Biochemistry, Jones and Bartlett Publishers, Boston, 1992.*
- *D. Voet, J. G. Voet, C. W. Pratt, Fundamentals of Biochemistry: Life at the Molecular Level, 4th Edition, 2012.*

PG Semester I

NCrF level	*6.0*
Title of the Course	*Advanced Physical Chemistry - I*
Course code	*CHMP-103*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop an advanced understanding of the principles governing chemical kinetics, phase equilibria, solid-state chemistry, surface phenomena, catalysis, and quantum chemistry.
- Explain the mechanisms and kinetics of complex chemical processes, including chain reactions, enzyme-catalyzed reactions, oscillatory reactions, and heterogeneous catalytic reactions.
- Apply thermodynamic and crystallographic principles to interpret phase behaviour, crystal structures, defects, and the physical properties of solid materials.
- Understand the relationship between surface properties, adsorption phenomena, and catalytic activity in chemical and industrial processes.
- Apply the principles of quantum mechanics to describe atomic and molecular structure, chemical bonding, spectroscopy, and electronic properties of matter.
- Develop analytical, mathematical, and problem-solving skills to interpret advanced concepts in physical chemistry and apply them to research and interdisciplinary scientific applications.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the mechanisms and kinetics of chain reactions, enzyme-catalyzed reactions, oscillatory reactions, and fast reactions using advanced kinetic models.

CO2: Apply Gibbs phase rule, Clausius–Clapeyron equation, and phase diagrams to analyze equilibrium behaviour in one- and two-component systems.

CO3: Interpret crystal structures using crystallographic principles, explain the role of defects and non-stoichiometry, and correlate structural features with the electrical, thermal, magnetic, and superconducting properties of solids.

CO4: Analyze adsorption phenomena, surface energetics, adsorption isotherms, and heterogeneous catalytic mechanisms, and evaluate their applications in chemical and industrial processes.

CO5: Apply the postulates of quantum mechanics, operator formalism, and approximate methods to solve problems related to atomic and molecular systems.

CO6: Explain molecular electronic structure using Molecular Orbital Theory, Valence Bond Theory, and Hückel Molecular Orbital Theory, and interpret bonding and electronic properties of molecules.

Unit I Advanced Chemical Kinetics ***Lecture Marks 10***

Chain reactions: General treatment and explanation of explosions; reaction mechanism and kinetics of H_2-Br_2 reaction and pyrolysis of alkane.

Enzyme catalysis: Mechanism and kinetics of enzyme catalysis reaction

Oscillatory reactions: Mechanism and kinetics. Reactions in flow systems; kinetics of fast reactions.

Unit II Phase Equilibria ***Lecture Marks 10***

Concept of phases, components, and degrees of freedom; derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour, and solid-vapour equilibria; Phase diagram of one-component systems (water and sulphur) and two-component systems (silver-lead and KI-H_2O)

Unit III Advanced Solid State ***Lecture Marks 15***

Types of solids; Order - spatial, orientational; Symmetry in crystals - primitive lattice vector–Wigner-Seitz cell - crystal systems - Bravais lattices - crystallographic point groups and space groups; X-ray diffraction - systematic absences - reciprocal lattice - Ewald construction - structure factor - crystal structure solution and refinement - common crystal structure motifs; quasicrystals. Point, line and plane defects; Intrinsic and extrinsic defects - vacancies, Schottky and Frenkel defects - charge compensation; Nonstoichiometry and defects - thermodynamic and structural aspects; Color centres. Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conduction. Free electron theory - electrical conductivity and Ohm's law - Hall effect; Energy bands - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; p-n junctions; Semiconductor/metal transition; Superconductivity- Meissner effect- type I and II superconductors- isotope effect- basic concepts of BCS theory- manifestations of the energy gap- Josephson devices.

Unit IV Surface Chemistry and Catalysis ***Lecture Marks 15***

Adsorption: Physical adsorption, chemisorption, nature of the adsorbed state; thermodynamics of adsorption; factors affecting adsorption.

Adsorption from solution: surface tension and surface free energy, application of surface tension, capillary action: Young-Laplace equation; formation of bubbles: Kelvin equation. Capillary condensation; adsorption in micropores and hysteresis loop; Gibbs adsorption equation; surface active and surface inactive materials.

Adsorption isotherms: Freundlich isotherm, Langmuir isotherm and BET isotherm; determination of the surface area of an adsorbent (Langmuir and BET equation); isosteric enthalpy of adsorption.

Catalytic activity at surfaces: mechanism of surface reaction; Langmuir-Hinshelwood and Eley-Rideal model; kinetic effects of surface heterogeneity and interactions. Kinetics of heterogeneous catalysis: unimolecular and bimolecular surface reactions.

Unit V- Revision Quantum Chemistry ***Lecture Marks 20***

Postulates of quantum mechanics, Operator algebra, Properties of hermitian operators, Eigenvalue problem, Commutators and Uncertainty Principle, Elementary applications of quantum mechanics-unbound motion in one dimension, Tunneling, Bound motion– particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor, Angular momentum algebra- Hydrogen atom, Methods of obtaining approximate solution to the time independent Schrödinger equation–perturbation theory and variational method, Application: Many electron atoms. Spin and Pauli exclusion principle, Hund’s rule. Slater determinants, Electronic term symbols. Born- Oppenheimer approximation, LCAO-MO and VB treatment of the Hydrogen molecule and Hydrogen molecule ion, Comparison of Molecular Orbital and Valence Bond Methods. Huckel molecular orbital theory: Postulates, application to ethylene, butadiene, and benzene. Introduction to extended Huckel theory

Suggested reading

- *Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry, 11th Ed., Oxford University Press, New Delhi (2018).*
- *Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., Physical Chemistry, 4th Ed., Wiley India, New Delhi (2006).*
- *Levine, I. N., Physical Chemistry, 6th Ed. McGraw Hill Education, New Delhi (2011).*
- *Laidler, K. J., Chemical Kinetics, 3rd Ed., Pearson Education, New Delhi (2011).*
- *Kapoor, K. L., A Textbook of Physical Chemistry: States of Matter and Ions in Solution, Vol. I, 6th Ed., McGraw Hill Education India (2019).*
- *Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry; 47th Ed, Vishal Publishing, New Delhi (2017).*
- *Adamson, A. W.; Gast, A. P., Physical Chemistry of Surfaces, 6th Ed, Wiley India, New Delhi (2011).*
- *Shaw, D. J., Introduction to Colloid and Surface Chemistry, 4th Ed, Butterworths Heinemann, Oxford (1992).*
- *Moudgil, H. K., Textbook of Physical Chemistry, PHI Learning, New Delhi (2010).*
- *Chandra, A. K., Introductory Quantum Chemistry, 4th Ed., McGraw Hill Education India, New Delhi (2017).*
- *Levine, I. N., Quantum Chemistry, 7th Ed., Pearson Education India, New Delhi (2016).*
- *McQuarrie, D. A., Quantum Chemistry, Viva Books, New Delhi (2016).*
- *Lewers, E. G., Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York (2011). 5. Jensen, F., Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell, New Jersey (2017).*
- *Sen, B. K., Quantum Chemistry Including Spectroscopy, 2nd Ed., Kalyani Publishers, New Delhi (2004).*
- *Atkins, P. W., Friedman R. S., Molecular Quantum Mechanics, 5th Ed., Oxford University Press, New Delhi (2012).*
- *Prasad, R. K., Quantum Chemistry, 4th Ed., New Age International Publishers, New Delhi (2010).*

PG Semester I

NCrF level	*6.0*
Title of the Course	*Research Methodology in Natural Sciences*
Course code	*CHMP-104*
Paper credit	*04* (L 3 – T 1 - P 0)
Total Contact Hours	*45 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After completing this course, students will be able to

- Understand the philosophy and importance of scientific research.
- Formulate research questions and testable hypotheses.
- Design experiments using appropriate scientific methods.
- Perform literature surveys using scientific databases.
- Apply statistical tools for data analysis and interpretation.
- Write scientific reports, research papers, dissertations and project proposals.
- Understand research ethics, plagiarism, intellectual property rights and publication ethics.

Course Outcomes (COs)

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

CO1: Explain the principles and philosophy of scientific research.

CO2: Identify research problems and formulate hypotheses.

CO3: Design scientific experiments using appropriate methodologies.

CO4: Analyze and interpret scientific data using statistical tools.

CO5: Prepare scientific manuscripts, dissertations and research proposals.

CO6: Demonstrate ethical conduct in research and scientific publication.

UNIT I: Foundations of Scientific Research *(8 Hours)*

Nature and philosophy of scientific research: Definition, objectives, significance, characteristics, scientific thinking, scientific temper.

Types of research: Basic research, applied research, translational research, interdisciplinary research, multidisciplinary research, qualitative research, quantitative research.

Scientific method: Observation, problem identification, hypothesis, experimentation, data collection, analysis, interpretation, conclusion, theory development.

Research problem: Identification, selection, feasibility, scope, novelty, significance, research gap.

Research hypothesis: Definition, characteristics, formulation, null hypothesis, alternative hypothesis, hypothesis testing.

Variables in research: Independent variable, dependent variable, controlled variable, confounding variable, operational definition.

Research design: Exploratory research, descriptive research, analytical research, experimental research, survey research.

Reliability and validity: Internal validity, external validity, reliability, reproducibility, repeatability.

UNIT II: Literature Survey and Research Planning *(8 Hours)*

Scientific literature: Primary literature, secondary literature, tertiary literature, review articles, books, monographs, conference proceedings, technical reports, patents.
Literature search: Keywords, Boolean operators, search strategies, advanced search techniques.
Scientific databases: Google Scholar, Scopus, Web of Science, ScienceDirect, PubMed, SpringerLink, Wiley Online Library, ACS Publications.
Bibliographic tools: Mendeley, Zotero, EndNote, citation management, reference organization.
Citation metrics: Citation index, impact factor, h-index, i10-index, journal ranking, quartile ranking.
Literature review: Critical analysis, synthesis of literature, identification of research gaps, conceptual framework.
Research proposal: Title, objectives, hypothesis, methodology, work plan, expected outcomes, budget estimation, timeline.

UNIT III: Experimental Design and Data Collection *(8 Hours)*

Experimental design: Objectives, variables, controls, replication, randomization, blocking.
Sampling techniques: Random sampling, systematic sampling, stratified sampling, cluster sampling, purposive sampling.
Sample size: Statistical considerations, confidence level, power of study.
Laboratory practices: Good Laboratory Practices (GLP), laboratory notebook, documentation, record keeping.
Measurement: Accuracy, precision, sensitivity, selectivity, uncertainty, calibration, validation.
Experimental errors: Systematic errors, random errors, gross errors, error minimization.
Quality assurance: Quality control, standard operating procedures (SOP), validation protocols.
Data collection: Experimental observations, instrumental measurements, field observations, questionnaires, surveys.

UNIT IV: Statistical Methods in Scientific Research *(8 Hours)*

Data classification: Qualitative data, quantitative data, discrete data, continuous data.
Descriptive statistics: Mean, median, mode, range, variance, standard deviation, coefficient of variation.
Probability concepts: Probability distribution, normal distribution, binomial distribution, Poisson distribution.
Statistical inference: Confidence interval, confidence level, sampling distribution.
Hypothesis testing: Null hypothesis, alternative hypothesis, p-value, significance level, Type I error, Type II error.
Statistical tests: Student's t-test, paired t-test, Chi-square test, F-test, one-way ANOVA.
Correlation and regression: Pearson correlation, Spearman correlation, linear regression, coefficient of determination.
Data visualization: Tables, graphs, histograms, scatter plots, bar charts, line graphs, box plots.
Software applications: MS Excel, R software, SPSS, Origin, GraphPad Prism.

UNIT V: Scientific Writing and Publication *(7 Hours)*

Scientific communication: Research paper, review article, technical report, thesis, dissertation, project report.
Research paper structure: Title, abstract, keywords, introduction, materials and methods, results, discussion, conclusion, references.
Scientific writing: Clarity, precision, objectivity, logical organization, technical language.
Tables and figures: Preparation, formatting, captions, graphical presentation, image quality.
Referencing styles: APA, MLA, Chicago, ACS, IEEE, Vancouver.
Scientific journals: Journal selection, indexing, open-access journals, subscription journals, predatory journals.

Publication process: Manuscript submission, editorial screening, peer review, revision, acceptance, publication.
Research communication: Oral presentation, poster presentation, seminar presentation, conference participation.
Research identifiers: DOI, ORCID, ResearcherID, Scopus Author ID.

UNIT VI: Research Ethics and Intellectual Property Rights (6 Hours)

Research ethics: Principles, integrity, accountability, transparency, responsible conduct of research.
Scientific misconduct: Fabrication, falsification, plagiarism, duplicate publication, salami publication, data manipulation.
Authorship ethics: Authorship criteria, corresponding author, acknowledgements, contributorship.
Conflict of interest: Financial conflict, academic conflict, disclosure policy.
Plagiarism: Types, detection methods, plagiarism checking software, prevention strategies.
Intellectual Property Rights (IPR): Copyright, patent, trademark, industrial design, geographical indication, trade secret.
Patent system: Patentability, patent application, patent filing, patent search, patent examination.
Technology transfer: Innovation, commercialization, licensing, entrepreneurship, startup ecosystem.
Research safety: Laboratory safety, biosafety, chemical safety, waste management, environmental safety.
Research governance: Institutional Ethics Committee (IEC), Institutional Animal Ethics Committee (IAEC), Institutional Biosafety Committee (IBSC), Human Ethics Committee, regulatory guidelines.

Practical / Tutorial Component

- Literature survey using Google Scholar and Scopus.
- Searching scientific journals and patents.
- Using Mendeley/Zotero for reference management.
- Preparation of a research proposal.
- Scientific paper review and presentation.
- Statistical analysis using MS Excel/R.
- Graph plotting and regression analysis.
- Detection of plagiarism using plagiarism-checking software.
- Preparation of a scientific poster.
- Oral seminar presentation.
- Writing a research article in IMRAD format.
- Preparation of a dissertation synopsis.

Suggested readings

- Kothari, C. R., & Garg, G. (2019). *Research Methodology: Methods and Techniques* (4th ed.). New Age International Publishers.
- Soumitro Banerjee (2021), *Research Methodology for Natural Sciences*, IISc Press / World Scientific
- Creswell, J. W., & Creswell, J. D. (2023). *Research Design: Qualitative, Quantitative, and Mixed Methods Approaches* (7th ed.). Sage Publications.
- Miller, J. N., & Miller, J. C. (2018). *Statistics and Chemometrics for Analytical Chemistry* (7th ed.). Pearson.
- Alley, M. (2018). *The Craft of Scientific Writing* (4th ed.). Springer.

N.B. Student can take similar MOOCs course available online in NPTEL/SWAYAM; https://nptel.ac.in/courses/127106227

PG Semester I

NCrF level	*6.0*
Title of the Course	*Advanced Interdisciplinary Chemistry Practical*
Course code	*CHMP-105*
Paper credit	*02* (L 0 – T 0 - P 2)
Total Contact Hours	*60 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop practical skills in the physicochemical and analytical characterization of environmental samples using standard analytical methods.
- Synthesize environmentally benign nanomaterials and functional materials using green chemistry principles and evaluate their applications.
- Perform laboratory experiments related to materials chemistry, nanotechnology, and environmental remediation using modern experimental techniques.
- Interpret experimental observations, analyze laboratory data, and prepare scientific reports following good laboratory practices.
- Develop problem-solving abilities, laboratory ethics, teamwork, and scientific communication skills required for research and industrial laboratories.

Course Outcomes (COs)

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

CO1: Perform physicochemical and analytical investigations of environmental samples using standard laboratory methods and interpret the results with reference to national and international standards.

CO2: Synthesize nanomaterials, biodegradable polymers, conducting polymers, and coordination compounds using conventional and green chemistry approaches and evaluate their physicochemical properties.

CO3: Apply spectroscopic, electrochemical, adsorption, and magnetic characterization techniques for the analysis of advanced materials and environmental samples.

CO4: Analyze experimental data, interpret scientific observations, and prepare laboratory reports using appropriate analytical and statistical methods while adhering to Good Laboratory Practices (GLP).

CO5: Demonstrate professional competence in laboratory safety, green chemistry principles, teamwork, ethical scientific practices, and effective scientific communication required for multidisciplinary research and industrial applications.

Unit I Environmental and Analytical Chemistry *(20 Hours)*

Students shall perform **any two** experiments.

- Physicochemical analysis of drinking water according to WHO/BIS standards: determination of pH, electrical conductivity, total dissolved solids (TDS), dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), total hardness, chloride, nitrate, and fluoride.
- Estimation of heavy metals in water or soil samples using UV–Visible spectrophotometry or colorimetric methods.
- Determination of phosphate and nitrate in natural water samples.

- Extraction and identification of microplastics from environmental water samples.
- Preparation of activated carbon from agricultural waste and evaluation of its adsorption efficiency for organic dyes.

Unit II: Green Chemistry and Sustainable Technologies *(20 Hours)*

Students shall perform **any two** experiments.

- Green synthesis and characterization of silver nanoparticles using plant extracts.
- Eco-friendly synthesis and characterization of ZnO nanoparticles.
- Catalytic degradation of organic dyes using synthesized nanoparticles.
- Preparation and characterization of biodiesel from waste cooking oil.
- Preparation and characterization of biodegradable polymer films using starch or chitosan.

UNIT III: Materials Chemistry and Nanotechnology *(20 Hours)*

Students shall perform **any two** experiments.

- Preparation and characterization of conducting polymers (Polyaniline or Polypyrrole).
- Sol–gel synthesis and characterization of silica nanoparticles.
- Fabrication of thin films using dip-coating or spin-coating techniques.
- Preparation and electrochemical characterization of supercapacitor electrode materials.
- Synthesis and characterization of coordination compounds and determination of magnetic susceptibility.

Suggested Readings

1. A. K. De, *Environmental Chemistry*, New Age International Publishers.
2. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, Cengage Learning.
3. P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press.
4. C. N. R. Rao, A. Müller and A. K. CHMEtham (Eds.), *The Chemistry of Nanomaterials*, Wiley-VCH.
5. J. B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing House.

Suggested Assessment Pattern

Total Marks: 100

Internal Assessment (30 Marks)		*End-Semester Practical Examination (70 Marks)*	
Component	***Marks***	***Component***	***Marks***
Continuous laboratory performance	*10*	*Practical experiment (one experiment)*	*25x2=50*
Laboratory notebook/record	*10*	*Observation, calculations and data interpretation*	*10*
Internal viva-voce and laboratory discipline	*10*	*Viva-voce*	*10*
Total	***30***	*Total*	*70*

PG Semester II

NCrF level	*6.0*
Title of the Course	*Advanced Inorganic Chemistry - II*
Course code	*CHMP-201*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop an advanced understanding of organometallic compounds, bioinorganic systems, inorganic solids, cluster chemistry, inorganic polymers, and the applications of group theory in inorganic chemistry.
- Explain the synthesis, bonding, structure, reactivity, and applications of metal carbenes, metallocenes, inorganic clusters, boranes, and inorganic polymers using modern bonding theories.
- Understand the structural and functional roles of metal ions and metalloenzymes in important biological processes and their significance in bioinorganic chemistry.
- Apply crystallographic principles to interpret the structures and properties of important ionic solids and correlate lattice energy with their physical and chemical behaviour.
- Apply group theoretical concepts to predict molecular symmetry, construct molecular orbitals, interpret spectroscopic transitions, and analyze chemical bonding in polyatomic molecules and coordination compounds.
- Develop analytical and problem-solving skills for interpreting structural, spectroscopic, and bonding aspects of advanced inorganic compounds relevant to research and industrial applications.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the synthesis, structure, bonding, reactivity, and applications of metal carbenes, carbynes, Tebbe's reagent, ferrocene, and other metallocenes using modern organometallic concepts.

CO2: Describe the structure, catalytic functions, and reaction mechanisms of biologically important metalloenzymes and metalloproteins involved in photosynthesis, nitrogen fixation, oxidation–reduction reactions, and vitamin B_{12}-dependent processes.

CO3: Explain the crystal structures of important ionic solids, evaluate the significance of lattice enthalpy, and correlate crystal structure with material properties.

CO4: Analyze the structure, bonding, electron counting, synthesis, and reactivity of metal carbonyl clusters, boranes, carboranes, metalloboranes, and Zintl ions using Wade's rules and isolobal analogy.

CO5: Explain the classification, synthesis, bonding, structure, and applications of inorganic polymers, including sulphur–nitrogen compounds, siloxanes, silicates, aluminosilicates, zeolites, and clays.

CO6: Apply group theoretical methods, including direct product representations, projection operators, and symmetry-adapted linear combinations (SALCs), to analyze molecular symmetry and chemical bonding.

CO7: Construct molecular orbital diagrams for polyatomic molecules and coordination compounds, predict spectroscopic selection rules, hybridization patterns, and electronic structures using group theory.

Unit I Advanced Organometallic chemistry — *Lecture/Marks: 15*

Metal carbenes: Introduction to metal-carbon multiple bonds, classifications, Fischer carbene, Schrock carbene, (Synthesis, Structure, bonding, synthesis and application), Tebb's reagent, metal carbynes

Ferrocene: Preparation and reactions (acetylation, alkylation, nitration and halogenation, metallation, Mannich condensation). Structure and aromaticity, Comparison of aromaticity and reactivity with that of benzene, other metallocenes

Unit II Advanced Bioinorganic Chemistry — *Lecture/Marks: 10*

Photosynthesis: reaction pathway, role of magnesium ions
Active site structure and activity of nitrogenase enzyme, xanthine oxidase, alcohol dehydrogenase, aldehyde oxidase, aldehyde dehydrogenase and V-B_{12}

Unit III Inorganic solids — *Lecture/Marks: 10*

Characteristic structure types of ionic solids: CsCl, NaCl, Spalerite and Wurtzite types of ZnS, fluorite and anti-fluorite, nickel arsenide, $CdCl_2$, CdI_2, rutile, perovskite and spinels, Lattice enthalpy, consequences of lattice enthalpy

Unit IV: Inorganic cluster, cage and polymer — *Lecture/Marks: 15*

Metal carbonyl clusters (low and high nuclearity clusters), calculation of metal-metal bond, electron counting in carbonyl clusters, binuclear clusters containing metel-metal multiple bonds, Metal-metal quadruple bond in $[Re_2Cl_8]^{2-}$, isolobal analogy, zintle ions, synthesis of carbonyl clusters
Structure and bonding in polyhedral boranes, carboranes, metalloboranes and metallocarboranes, *styx* notation; Wade's rule; electron count in polyhedral boranes; synthesis of polyhedral boranes.

Types of inorganic polymers, comparison with organic polymers, Synthesis, structure and bonding in sulphur-nitrogen compounds, siloxanes, iso- and hetero-poly anions, Structure and chemistry of silicates, aluminosilicates, zeolites and clays

Unit IV Applications of Group Theory — *Lecture/Marks: 20*

Direct product representation, projection operator and symmetry-adapted linear combination (SALC), symmetry selection rules for IR, Raman and electronic spectra. Hybrid orbital and hybridisation in polyatomic molecules, construction of hybrid orbitals for sigma & □-bonding (e.g. D3h, D4h, Td, Oh). Molecular Orbital Theory: LCAO-MO approach; Construction of MO diagrams of polyatomic molecules (e.g. BeH2, H2O, BH3, NH3, CH4) including coordination complexes (Oh and Td).

Suggested reading

- F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, Wiley.

- J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson.
- Miessler, Fischer & Tarr, *Inorganic Chemistry*, 5th Edition, Pearson.
- Gary L. Miessler, Paul J. Fischer & Donald A. Tarr, *Inorganic Chemistry*, Pearson.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J. & Armstrong, F., *Inorganic Chemistry*, Oxford University Press.
- Satya Prakash, G. D. Tuli, S. K. Basu & R. D. Madan, *Advanced Inorganic Chemistry*, S. Chand.
- P. L. Soni & Mohan Katyal, *Textbook of Inorganic Chemistry*, Sultan Chand & Sons.
- R. L. Dutta, *Inorganic Chemistry*, Part I & II, New Age International.
- Gurdeep Raj, *Advanced Inorganic Chemistry*, Goel Publishing House.
- B. R. Puri, L. R. Sharma & K. C. Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing Co.
- A. K. De, *A Textbook of Inorganic Chemistry*, New Age International.

PG Semester II

NCrF level	*6.0*
Title of the Course	*Advanced Organic Chemistry - II*
Course code	*CHMP-202*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

1. Develop an advanced understanding of organic photochemical and pericyclic reactions, including their mechanisms, stereochemical outcomes, and synthetic applications.
2. Explain the synthesis, structure, reactivity, and aromaticity of important heterocyclic compounds and correlate their chemical behaviour with electronic structure.
3. Analyze conformational and stereochemical aspects of organic molecules using modern stereochemical principles and chiroptical methods.
4. Apply contemporary synthetic methodologies involving organometallic reagents, selective reagents, and catalytic processes for efficient carbon–carbon and carbon–heteroatom bond formation.
5. Develop mechanistic reasoning and retrosynthetic skills for designing efficient synthetic routes to complex organic molecules.
6. Strengthen analytical and problem-solving abilities for interpreting reaction mechanisms, stereochemical behaviour, and modern synthetic transformations relevant to pharmaceutical, medicinal, and industrial chemistry.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the principles, mechanisms, and synthetic applications of organic photochemical and pericyclic reactions, including orbital symmetry and stereochemical selection rules.

CO2: Analyze the synthesis, aromaticity, electronic properties, and chemical reactivity of saturated and aromatic heterocyclic compounds, including fused and diazine systems.

CO3: Interpret conformational preferences, stereochemical effects, and chiroptical properties of organic molecules and correlate molecular structure with chemical reactivity.

CO4: Apply modern synthetic methodologies involving organopalladium coupling reactions, olefination reactions, and organometallic reagents for selective carbon–carbon bond formation.

CO5: Explain the role and synthetic applications of organosulphur compounds, enamines, hydroboration, organosilicon, organozinc, organocopper, and other selective reagents in advanced organic synthesis.

CO6: Predict reaction pathways, stereochemical outcomes, and product formation based on mechanistic principles and reagent selectivity.

CO7: Design efficient synthetic strategies using modern reagents, catalytic transformations, and retrosynthetic analysis for the synthesis of complex organic molecules.

Unit I Organic Photochemistry and Pericyclic Reactions — *Lecture Marks 20*

Introduction to organic photochemistry, electronic transitions, Laws of photochemistry, quantum yield; cis-trans isomerisation, Norrish Type I & II reactions, photoreduction of ketones, Paterno-Buchi reaction, Lumketone rearrangement, Di-π-methane and Di-π-methane type rearrangement, Aza-Di-π-methane type rearrangement, rearrangement of dienones and β,γ-unsaturated ketones.

Introduction; types of pericyclic reactions: electrocyclic reactions, cycloaddition, 1,3-dipolar addition, cheletropic reactions, sigmatropic and group transfer reactions; Ene reaction; selection rules; general orbital symmetry rules.

Unit II Advanced Heterocyclic Chemistry *Lecture Marks 15*

Syntheses of aziranes, oxiranes & thiiranes; ring openings and heteroatom extrusion; synthesis & reactions of azetidines, oxetanes & thietanes. Aromatic heterocycles: Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole. Concept of π-excessive and π-deficient heterocyclics. Condensed Five-membered Rings (1 Heteroatom): Synthesis and reactions of indole, benzofuran and benzothiophene. Diazines: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines, nucleophilic and electrophilic substitutions.

Unit III Advanced Stereochemistry *Lecture Marks 15*

Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl, 3-alkyl, and 4-alkyl ketone effects. A 1,2 and A 1,3 strains. Conformation of fused systems - decalins and perhydrophenanthrenes. Effects of conformation on reactivity and mechanism of basic organic reactions of 6-membered ring compounds. Chiroptical properties - Optical rotatory dispersion, circular birefringence, circular dichroism, axial haloketone rule, octane rule.

Unit IV Advanced Organic Synthesis *Lecture Marks 20*

Organometallic reagents in formation of carbon-carbon bonds: Organopalladium in C-C formation (Heck reaction, Stille, Suzuki, Sonogashira and Negishi Coupling). Formation of C=C bonds by elimination reactions, syn elimination; Wittig and related reactions, McMurry reaction, Peterson olefination, Julia reaction and Tebbe olefination. Use of organosulphur compounds for reversal of polarity (Corey-Seebach Umpolung). Allylic activation by - allyl Ni and – allyl Pd complexes.
Application of Enamines, Hydroboration and trialkylsilyl halides in organic synthesis. Use of the following reagents: Organotin (TBTH), Lithium Diisopropyl Amide (LDA), Dicyclohexylcarbodiimide, Dicyanodichloroquinone (DDQ), Dimethyl dioxirane (DDO), lipase and other reagents of organozinc and organocopper.

Suggested reading

- *Smith, M. B.; March, J., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley India, New Delhi (2015).*
- *Greeves, N.; Clayden, J.; Warren, S., Organic Chemistry, 2nd Ed., Oxford University Press, New Delhi (2012).*
- *Carruthers, W., Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, New Delhi (2005).*
- *Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, 3rd Ed., New Age International Publishers, New Delhi (2018).*
- *Sengupta, S., Basic Stereochemistry of Organic Molecules, 2nd Ed., Oxford University Press, New Delhi (2018).*
- *Kalsi, P. S., Stereochemistry: Conformation and Mechanism, 10th Ed., New Age International Publishers, New Delhi (2019).*

PG Semester II

NCrF level	*6.0*
Title of the Course	*Advanced Physical Chemistry- II*
Course code	*CHMP-203*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop an advanced understanding of chemical kinetics, thermodynamics, phase equilibria, and polymer chemistry through quantitative and molecular-level approaches.
- Explain the theories of reaction rates, reaction mechanisms, solvent effects, and the factors governing the kinetics of homogeneous reactions.
- Apply thermodynamic principles to describe non-ideal systems, phase transitions, partial molar properties, and chemical equilibria.
- Interpret phase diagrams of binary and ternary systems and apply distribution laws to extraction and separation processes.
- Understand the structure, molecular characteristics, polymerization mechanisms, and physicochemical behaviour of macromolecules.
- Develop analytical, mathematical, and problem-solving skills to explain physicochemical phenomena and apply them in research, industrial chemistry, and materials science.

Course Outcomes (COs)

After successful completion of the course, students will be able to:

CO1: Explain the principles of kinetic and thermodynamic control of reactions and evaluate reaction mechanisms using collision theory, transition state theory, and unimolecular reaction models.

CO2: Analyze the influence of solvent, ionic strength, dielectric constant, and diffusion on reaction rates and predict kinetic behaviour in solution-phase reactions.

CO3: Apply the concepts of fugacity, activity, chemical potential, Gibbs–Duhem equation, and partial molar properties to interpret the thermodynamic behaviour of ideal and non-ideal systems.

CO4: Interpret binary and ternary phase diagrams, explain eutectic and congruent/incongruent melting systems, and apply the Nernst distribution law to solvent extraction and related separation processes.

CO5: Explain the classification, molecular characteristics, polymerization mechanisms, and molecular weight determination methods of polymers and macromolecules.

CO6: Analyze the configuration, conformation, diffusion behaviour, and chain statistics of polymer molecules using appropriate theoretical models.

Unit-I Chemical Kinetics III *Lecture Marks 15*

Kinetic control and thermodynamic control of reaction, Theories of reaction rate: Arrhenius theory; simple collision theory (SCT); steric factor, activated complex theory (ACT); thermodynamics of reaction rate and entropy of activation. Theories of unimolecular reactions: Lindemann mechanism and Hinshelwood treatment.

Reaction in solution: diffusion-controlled and chemically controlled reaction; factors affecting reaction rate in solution; effect of solvent and ionic strength on the rate constant: primary and secondary salt effect; effect of the dielectric constant of the medium on the rate of reaction in solution.

Unit II Chemical Thermodynamics III *Lecture/Marks: 15*

Fugacity and activity and their variation with temperature and pressure, Graphical method for the determination of fugacity; fugacity of van der Waals gases

Partial molar quantities and their physical significance; Partial molar free energy (chemical potential) and its variation with temperature and pressure; Gibbs-Duhem equation

Gibbs free energy and entropy of mixing of ideal gases; partial molar volumes; method of determination of partial molar volumes, Thermodynamic description of phase transitions and Clapeyron-Clausius equation

Unit III Phase Equilibria-II *Lecture/Marks: 15*

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Three-component systems, water-chloroform-acetic acid system, triangular plots

Nernst distribution law and its limitations, thermodynamic derivation, Modification of distribution law to cases of association and dissociation of solute and complex formation, Application of the law in the process of extraction

Unit IV Macromolecules *Lecture Marks: 15*

Brief overview of polymers: Classification and types of polymers. Concept and types of molecular weight; distribution of molecular weight in polymers; significance of molecular weight; degree of polymerization and chain length, Methods of determining molecular weights of macromolecules: End group analysis; osmometry, viscometry and light scattering methods. Types of polymerization; kinetics of addition and step growth (condensation) polymerisation, Different models for describing the size and shape of dissolved macromolecules; configuration and conformation of macromolecules, Diffusion and Stokes-Einstein equation, Distribution of chain lengths: average end-to-end, root mean square end-to-end and most probable end-to-end chain length.

Suggested reading

- *Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry, 11th Ed., Oxford University Press, New Delhi (2018).*
- *Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., Physical Chemistry, 4th Ed., Wiley India, New Delhi (2006).*

- *Levine, I. N., Physical Chemistry, 6th Ed. McGraw Hill Education, New Delhi (2011).*
- *Laidler, K. J., Chemical Kinetics, 3rd Ed., Pearson Education, New Delhi (2011).*
- *Kapoor, K. L., A Textbook of Physical Chemistry: States of Matter and Ions in Solution, Vol. I, 6th Ed., McGraw Hill Education India (2019).*
- *Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry; 47th Ed, Vishal Publishing, New Delhi (2017).*
- *Kapoor, K. L., A Textbook of Physical Chemistry: Thermodynamics and Chemical Equilibrium, Vol. II, 6th Ed., McGraw Hill Education India (2019).*
- *Prigogine, I., Introduction to Thermodynamics of Irreversible Processes, 3rd Ed., Wiley (1968).*
- *Billmeyer, F. W., Textbook of Polymer Science, 3rd Ed., Wiley India, New Delhi (2007).*
- *Gowariker, V. R., Viswanathan, N. V. and Sreedhar, J., Polymer Science, 3rd Ed., New Age International Publishers, New Delhi (2019).*

PG Semester II

NCrF level	*6.0*
Title of the Course	*Advanced Chemistry Practical*
Course code	*CHMP-204*
Paper credit	*08* (L 0 – T 2 - P 6)
Total Contact Hours	*180 hours*
Distribution of Marks	*200 (End semester examination 140 + internal assessment 60)*

Course Objectives

After successful completion of this course, students will be able to:

- Perform advanced inorganic, organic and physical chemistry experiments independently.
- Synthesize and characterize coordination compounds, nanomaterials and organic molecules.
- Apply modern instrumental techniques such as UV–Visible spectroscopy, FTIR and TLC for qualitative and quantitative analysis.
- Analyse experimental data using statistical and computational tools.
- Interpret spectroscopic and kinetic data and prepare scientific laboratory reports.
- Demonstrate safe laboratory practices, research ethics and scientific communication skills.

Course Outcomes (COs)

Upon successful completion of the course, students will be able to:

CO1: Demonstrate proficiency in advanced laboratory techniques for inorganic, organic, and physical chemistry, including quantitative analysis, synthesis of coordination compounds, organic synthesis, kinetic studies, electrochemical measurements, and thermodynamic investigations.

CO2: Synthesize, purify, and characterize coordination compounds, nanomaterials, semiconductor materials, and organic compounds using appropriate experimental techniques and instrumental methods such as TLC, UV–Visible spectroscopy, FTIR spectroscopy, and other available analytical tools.

CO3: Analyze, interpret, and present experimental data using appropriate mathematical, statistical, and computational methods, including spreadsheet software (Excel/Origin/R), and apply scientific principles to solve chemical problems.

CO4: Apply research methodology, scientific literature survey, molecular visualization, laboratory safety practices, green chemistry principles, and good laboratory practices (GLP) in planning, executing, and documenting laboratory investigations.

CO5: Communicate scientific findings effectively through laboratory records, technical reports, research paper presentations, and oral discussions while demonstrating ethical conduct, teamwork, and professional competence required for research and industrial laboratories.

Part A Inorganic Chemistry Practical

Students shall perform any SIX experiments, including: One quantitative analysis, Three coordination/synthetic chemistry experiments, One nanomaterials or polyoxometallate experiment, One instrumental/computational experiment

- Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy etc.
- Solution phase synthesis of coordination compounds e.g. vanadylacetylacetonate, potassium trisoxalatometal(III) trihydrate etc.; characterization, properties and applications (e.g. catalysis).
- Synthesis of coordination compounds through ligand synthesis and spectroscopic characterization, e.g. preparation of bis(*N*,*N*-disalicylideneethylenediammine)(μ-aquadicobalt(II).
- Solid phase synthesis of coordination compounds (e.g. Reinecke salt, *trans*-bisglycinatocopper(II)) and their properties.
- Isomerism in coordination compounds. e.g. conversion of chloropentammine cobalt(III) chloride to nitro and nitroso isomers, *cis*- and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride etc.
- Preparation of metal(II) isonicotinatetetrahydrates, characterization, use as precursors to metal oxides.
- Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.
- Synthesis and characterization of semiconductor nanocrystals (CdS, ZnS, ZnO etc.).
- Preparation of polyoxometallates (e.g. tetrabutylammoniumhexamolybdate(VI)), characterization.
- Quantitative determination of components in food (Fe, Zn, I, Ca, etc.)
- Applications of UV–Visible spectroscopy: (a) Verification of Beer–Lambert's law, (b) Determination of composition of Fe(III)–salicylate complex by Job's method, (c) Kinetic study of the acetone–iodine reaction by colorimetry.

Part B Organic Chemistry Practical

Students shall perform any SIX experiments including at least one qualitative analysis, one estimation experiment, three synthetic experiments and one instrumental characterization experiment.

- Qualitative analysis : Binary mixture analysis (solid-solid, solid-liquid, liquid-liquid)
- Estimation of amino acids using titrimetric methods
- Estimation of sugars using titrimetric (redox) methods.
- Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using NaBH4.
- Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazophenanthrene derivative.
- Organic preparations involving two or more steps: (a) Benzopinacolone from benzophenone via benzopinacol (b) Benzilic acid from benzoin (c) Dibenzyl from benzoin (d) Anthranilic acid from phthalic anhydride (e) Any halogenation reaction etc. 2. Greener practice in organic synthesis: (a) Acetylation of primary amine (b) Bromination of acetanilide (c) Nitration of phenol (d) Pinacol Pinacolone rearrangement
- Multicomponent reaction of aldehyde, β–keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction)
- Multicomponent reaction of aldehyde, β–keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis)
- Extraction, purification and characterization of natural products (curcumin/caffeine/eugenol/limonene/chlorophyll) using TLC and UV–Visible spectroscopy.

Note: During all organic synthesis experiments, students shall monitor the progress of the reaction using Thin Layer Chromatography (TLC) with appropriate solvent systems and determination of Rf values. Synthesized compounds should be characterized, wherever applicable, using melting point determination, FTIR spectroscopy and UV–Visible spectroscopy.

Part C Physical Chemistry Practical

Students shall perform any SIX experiments covering chemical kinetics, electrochemistry, thermodynamics, surface chemistry and computer-assisted data analysis.

- Determination of the temperature coefficient and activation energy of acid hydrolysis of methyl acetate using the least squares method.
- Study of the kinetics of saponification of ethyl acetate by sodium hydroxide and determination of the rate constant and reaction order.
- Kinetics of the reaction between iodine and acetone in acidic medium and determination of the reaction order.
- Investigation of the kinetics of oxidation of ethanol by chromium(VI) and determination of the rate constant.
- Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's law and calculation of its dissociation constant.
- Conductometric titration of binary mixtures: $HCl + CH_3COOH$, $H_2SO_4 + CuSO_4$, $HCl + KCl$
- Potentiometric estimation of hydrochloric acid, acetic acid, and their binary mixture using standard sodium hydroxide.
- Potentiometric titration of ferrous ammonium sulphate with potassium dichromate and determination of the standard electrode potential of the Fe^{3+}/Fe^{2+} system.
- Adsorption of methylene blue on activated carbon and analysis using Langmuir and Freundlich adsorption isotherms.
- Determination of adsorption kinetics of dye on activated carbon.
- Determination of the critical micelle concentration (CMC) of a detergent by surface tension measurement.
- Determination of the heat capacity of a calorimeter and the enthalpy of solution of ammonium chloride.
- Determination of the Van't Hoff factor of an electrolyte by cryoscopic method.
- Determination of the solubility product of calcium hydroxide by studying its solubility in sodium hydroxide solution.
- Computer-assisted data analysis using least-squares fitting (linear and exponential plots) and determination of kinetic and thermodynamic parameters using spreadsheet software (Excel/Origin/R).

Tutorial Component (2 Credits)

Students shall complete at least two of the following tutorial activities

- Literature survey using SciFinder, Reaxys, PubChem and Web of Science.
- Research paper presentation and discussion.
- Interpretation of UV–Visible, IR, NMR and Mass spectra.
- Statistical analysis of experimental data using Excel, Origin or R.
- Laboratory safety, GLP and chemical waste management.
- Scientific report writing and referencing.
- Introduction to computational chemistry and molecular visualization.

The Department may introduce additional experiments or modify existing experiments from time to time in accordance with advances in chemical sciences and the availability of laboratory facilities, with the approval of the Board of Studies.

Books Recommended

- J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel‘s Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, 2009.
- G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis,Pearson Education, 7th Edition. 2013.
- Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R., Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, New Delhi (2003).
- Mann, F. G.; Saunders, B. C., Practical Organic Chemistry, 4th Ed., Pearson Education India, New Delhi (2009).
- Clarke, H. T., A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, New Delhi (2007).
- J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edison, 2008.
- J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, PragatiPrakashan, 6th Edition, 2014.
- M. Halpern, Experimental Physical Chemistry, 2nd Edition, Prentice Hall, Upper Saddle River, NJ 07458
- Other Sources: *Journal of Chemical Education*, ACS Publications.

Assessment Pattern (Total Marks: 200)

A. Continuous Internal Assessment *(60 Marks)*

Component	***Inorganic***	***Organic***	***Physical***	***Total***
Continuous laboratory performance	*10*	*10*	*10*	*30*
Laboratory record book	*5*	*5*	*5*	*15*
Viva during practical classes	*5*	*5*	*5*	*15*
Total	***20***	***20***	***20***	***60***

B. Tutorial Assessment *(40 Marks)*

Component	***Marks***
Literature survey/Scientific database search	*10*
Seminar/Research paper presentation	*10*
Spectral interpretation/Computational exercise/Data analysis	*10*
Scientific report writing/Assignment	*10*
Total	***40***

C. End Semester Practical Examination *(100 Marks)*

Each student performs ***one experiment from each branch****.*

Component	***Marks***
Inorganic Chemistry Practical	*25*
Organic Chemistry Practical	*25*
Physical Chemistry Practical	*25*
Comprehensive Viva-Voce (covering all three branches and tutorial topics)	*18*
Discipline/ team work/ cooperation	*07*
Total	***100***

PG Semester III

NCrF level	*6.5*
Title of the Course	*Advance Inorganic Chemistry - III*
Course code	*CHMP-301*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Understand the mechanisms of electron transfer reactions, ligand substitution, molecular rearrangements and stereochemical transformations in coordination compounds.
- Explain the mechanistic pathways of organometallic reactions and homogeneous catalytic processes employed in modern chemical synthesis and industrial applications.
- Develop a comprehensive understanding of advanced spectroscopic techniques such as NMR, ESR, Mössbauer and NQR spectroscopy for structural and electronic characterization of inorganic and organometallic compounds.
- Correlate spectroscopic parameters with molecular structure, bonding, oxidation state, electronic configuration and magnetic properties.
- Apply mechanistic and spectroscopic concepts to interpret experimental observations and solve advanced inorganic chemistry problems.
- Appreciate the role of modern inorganic spectroscopy and catalysis in contemporary research, materials science and bioinorganic chemistry.

Course Outcomes (COs)

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

CO1: Explain the mechanisms of electron transfer, substitution, isomerization, racemization and ligand-centred reactions in coordination chemistry.

CO2: Interpret the mechanisms of oxidative addition, reductive elimination, migratory insertion, β-hydride elimination and related organometallic transformations involved in homogeneous catalysis.

CO3: Analyse important industrial catalytic processes including alkene hydrogenation, hydroformylation, Wacker oxidation, Monsanto acetic acid process, Fischer–Tropsch synthesis, olefin metathesis and Ziegler–Natta polymerization.

CO4: Interpret multinuclear NMR spectra (^{1}H, ^{19}F, ^{31}P and ^{11}B) of inorganic and organometallic compounds for structural characterization.

CO5: Analyse ESR spectra of transition metal complexes, inorganic radicals and biologically important paramagnetic species by correlating spectral parameters with electronic structure.

CO6: Explain the principles, instrumentation and applications of Mössbauer and Nuclear Quadrupole Resonance (NQR) spectroscopy in the characterization of inorganic compounds.

CO7: Correlate spectroscopic data with bonding, oxidation state, coordination geometry, magnetic behaviour and molecular symmetry in inorganic systems.

Unit I Electron transfer reaction — *Lecture/Marks: 15*

Rearrangement of Precursor complex and electron transfer; Nature of bridging ligand; 2-electron transfer; Synthesis of coordination compounds using redox reaction; complementary and non-complementary reaction; Oscillating reactions; Template effect and macrocyclic ligands; reactions of coordinated ligands. Synthesis of coordination compounds by substitution reactions; Isomerization and racemization of tris chelate complexes; Molecular rearrangement in four-coordinated and six-coordinated complex.

Unit II Advanced Organometallic Chemistry — *Lecture/Marks: 20*

Mechanism of oxidative addition, intramolecular addition, addition to multiple bond, oxidative coupling, salient feature of reductive elimination, migratory insertion (mechanism and evidence), insertion of alkenes, beta-hydrogen elimination and alpha-hydrogen abstraction

Introduction to catalytic cycles, TON and TOF
Homogeneous organometallic catalysis: alkene hydrogenation using Wilkinson catalyst; hydroformylation of olefins using cobalt or rhodium catalyst; oxidation of olefins by Wacker method; Monsanto acetic acid process; olefin oligomerisation, metathesis and isomerisation, Fischer-Tropsch reaction, Ziegler-Natta olefin polymerisation.

Unit III Inorganic NMR and ESR — *Lecture/Marks: 20*

NMR Spectroscopy: Proton NMR spectra of metal hydride complexes, NMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple inorganic and organometallic compounds.

Characteristic features of ESR spectra, line shapes and line widths; ESR spectrometer. The g value and the hyperfine coupling parameter (A), origin of hyperfine interaction. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals. ESR spectra of magnetically dilute samples.

Unit IV Mossbauer and NQR spectroscopy — *Lecture/Marks: 15*

Mossbauer spectroscopy: Principle of Mossbauer spectroscopy, Instrumentation, Application of Mossbauer spectroscopy: the isomer shift, magnetic interaction, quadruple splitting, line width. Application to iron-to-iron and tin compounds,

NQR spectroscopy: Principle of NQR, Quadruple constant, Application of NQR spectroscopy.

Suggested readings

- F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann – Advanced Inorganic Chemistry
- J. E. Huheey, E. A. Keiter and R. L. Keiter – Inorganic Chemistry: Principles of Structure and Reactivity
- R. H. Crabtree – The Organometallic Chemistry of the Transition Metals
- R. S. Drago – Physical Methods in Chemistry

PG Semester III

NCrF level	*6.5*
Title of the Course	*Advanced Organic Chemistry III*
Course code	*CHMP-302*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course objectives

After successful completion of this course, students will be able to:

- Comprehend the chemistry of enols, enolates and related carbon nucleophiles, and their applications in carbon-carbon bond-forming reactions.
- Enlighten the mechanisms, stereochemical aspects and synthetic significance of important named organic reactions and molecular rearrangements.
- Develop a comprehensive understanding of physical organic principles governing reaction mechanisms, including kinetics, thermodynamics, catalysis, isotope effects and solvent effects.
- Correlate mechanistic concepts with experimental evidence to elucidate reaction pathways, intermediates and transition states in organic reactions.
- Apply the principles of protecting group chemistry and retrosynthetic analysis for the rational design and execution of multistep organic syntheses.
- Appreciate the importance of modern synthetic methodologies and mechanistic reasoning in advanced organic synthesis and research.

Course outcomes (COs)

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

CO1: Explain the generation, structure and reactivity of enolates, dianions and related enolate equivalents, and analyse factors governing regioselectivity, chemoselectivity and kinetic versus thermodynamic control in alkylation reactions.

CO2: Interpret the mechanisms and synthetic applications of Michael addition, conjugate addition, conjugate substitution and Robinson annulation, including reactions involving organometallic reagents and silicon-based nucleophiles.

CO3: Analyse the mechanisms, stereochemical features and synthetic significance of important named reactions, including Mukaiyama aldol, Darzens, Mannich, Shapiro, Julia olefination, Peterson elimination, Wolff, Curtius, Hofmann, Schmidt, Beckmann rearrangements, Baldwin's rules, Barton reactions, McMurry coupling, Birch reduction and Lindlar reduction.

CO4: Explain the principles of physical organic chemistry by correlating reaction kinetics, thermodynamic stability, Hammond's postulate, Curtin-Hammett principle, catalysis, isotope effects and solvent effects with organic reaction mechanisms.

CO5: Apply experimental approaches, including kinetic studies, isotopic labelling and kinetic isotope effects, to identify reaction intermediates, transition states and mechanistic pathways.

CO6: Interpret the principles of protection and deprotection of functional groups, and apply chemo-, regio- and stereoselective strategies in multistep organic synthesis.

CO7: Apply retrosynthetic analysis using synthons, disconnections, functional group interconversions, umpolung and carbon-carbon bond disconnection strategies for the design of efficient synthetic routes to target molecules.

CO8: Critically evaluate mechanistic and retrosynthetic approaches for solving complex synthetic problems and apply advanced concepts of organic synthesis to research-oriented and industrial applications.

Unit I Enol and enolate Chemistry — *Lecture Marks 25*

Alkylation of carbon *via* enolates and specific enolate equivalents: Generation of carbon nucleophiles by proton abstraction, kinetic *vs* thermodynamic control in formation of enolates, alkylation of enolates, generation and alkylation of dianions, solvent effect in enolate alkylations, oxygen vs carbon as the site of alkylation, alkylation of aldehydes, esters, lactones and nitro compounds, use of enol derivatives (enamines, vinyl acetates, vinyl-silyl-ethers, C- or O-Sn- derivatives, boron aluminium enolates). Michael addition: 1,2- *vs* 1,4-addition, conjugate addition followed by alkylation, conjugate substitution reactions (Baylis-Hilmann reaction, nucleophilic epoxidation), conjugate addition of organometallic reagents such as Cu-derivatives (Gilman reagents), Grignard reagents, improvements of the Robinson annulation with alpha-silyl methylvinyl ketone use of vinyl pyridine, Micahel addition of vinyl-silyl-ethers and allylsilanes.

Unit II Some important name reactions — *Lecture Marks 15*

Mukaiyama aldol reaction, Darzen reaction, Mannich reaction, Shapiro reaction, McMurry reaction, Julia olefination, Peterson elimination, Wolff rearrangement, Curtius, Hoffmann, Schmidt, Beckmann rearrangement, Baldwin's rules, Barton deoxygenation and decarboxylation, McMurry coupling, Birch reduction and Lindlar's reduction.

UNIT III Determination of reaction mechanism — *Lecture Marks 15*

Physical organic chemistry: Relationship between thermodynamic stability and rates of reactions – kinetic and thermodynamic control of product formation, Hammond's postulate, Curtin Hammett principle. Catalysis (acids, bases, and nucleophiles) and isotope effects, importance in the determination of organic reaction mechanisms, solvent effects, examples from S_N2 and E2 reactions. Detection of transition state and intermediates, labeling and kinetic isotope effects.

Unit IV Protection-deprotection and Retrosynthesis — *Lecture Marks 15*

Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

Retrosynthetic analysis: Synthesis backwards, disconnections, synthons (donor and acceptor), choosing disconnections, functional group interconversion, disconnection approach of alcoholic and keto compound, C–C disconnections, natural reactivity and umpolung. Protective groups (hydroxyl, amine, carbonyl and carboxylic and C-C double bond protecting groups) in organic synthesis.

Suggested Readings

- *Clayden, J., Greeves, N., & Warren, S. Organic Chemistry (3rd ed.). Oxford University Press, 2021.*

- *Solomons, T. W. G., Fryhle, C. B., & Snyder, S. A. Organic Chemistry (13th ed.). John Wiley & Sons, 2023.*
- *Warren, S., Organic Synthesis: The Disconnection Approach, Wiley India, New Delhi (2007).*
- *Bruice, P. Y. Organic Chemistry (8th ed.). Pearson Education, 2016.*
- *Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (8th ed.). Wiley, 2020.*
- *Carey, F. A., & Sundberg, R. J. Advanced Organic Chemistry, Part B: Reactions and Synthesis (5th ed.). Springer, 2007.*

PG Semester III

NCrF level	*6.5*
Title of the Course	*Advanced Physical Chemistry - III*
Course code	*CHMP- 103*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of non-equilibrium thermodynamics and its application to irreversible physical and chemical processes.
- Understand the principles of statistical thermodynamics and establish the relationship between microscopic molecular behaviour and macroscopic thermodynamic properties.
- Apply quantum mechanical methods to describe atomic and molecular systems using approximate theoretical approaches.
- Explain many-electron quantum mechanical methods and computational techniques employed in modern theoretical chemistry.
- Develop the ability to interpret molecular structure, electronic properties and reaction mechanisms using computational chemistry.
- Acquire the theoretical foundation required for advanced research in physical chemistry, quantum chemistry and molecular modelling.

Course Outcomes (COs)

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

CO1: Explain the principles of non-equilibrium thermodynamics, entropy production, thermodynamic forces and fluxes, and irreversible transport phenomena.

CO2: Apply statistical thermodynamic concepts, ensemble theory and partition functions to evaluate thermodynamic properties of atomic and molecular systems.

CO3: Analyse molecular systems using approximation methods such as the variational method, perturbation theory, Born–Oppenheimer approximation and self-consistent field approaches.

CO4: Explain the theoretical basis of many-electron quantum mechanics, Hartree–Fock theory, Slater determinants and related computational methods.

CO5: Interpret electronic structures, molecular geometries, thermochemical properties and reaction pathways using quantum chemical calculations.

CO6: Evaluate the principles, advantages and limitations of semi-empirical, *ab initio* and density functional theory (DFT) methods for computational investigations.

CO7: Apply computational chemistry techniques for geometry optimization, transition-state analysis and prediction of molecular properties relevant to chemical research.

CO8: Critically analyse theoretical and computational results and integrate thermodynamic and quantum mechanical concepts for solving advanced problems in physical chemistry.

Unit I Non-Equilibrium Thermodynamics *Lecture Marks 15*

Difference between equilibrium and non-equilibrium thermodynamics, Postulates of non-equilibrium thermodynamics; Curie-Prigogine principle and microscopic reversibility, Onsagar's relations: thermodynamic and kinetics point of view; phenomenological laws.

The entropy of irreversible processes: Clausius inequality; entropy production due to heat flow, mass flow, chemical reactions and electrochemical reactions; rate of entropy productions-generalized fluxes and forces; thermodynamic forces and fluxes; the relation between forces and fluxes; Thermoelectric phenomenon: Peltier, Seebeck and Thomson effect. Relation between chemical potential and thermodynamic potentials

Unit II Statistical Thermodynamics *Lecture Marks 15*

Concepts of statistical thermodynamics, entropy and thermodynamic probability, Different types of ensembles, ensemble averaging; Stirling approximation, Distribution laws: Maxwell–Boltzmann, Fermi–Dirac and Bose-Einstein; limitation of applicability of various distribution laws

Partition function and its properties, thermodynamic properties in terms of partition functions, evaluation of translational, rotational, vibrational, electronic and nuclear partition functions; law of equipartition of energies; and heat capacity.

Unit III Quantum Mechanical Applications-I *Lecture Marks 12*

Variation theorem and linear variation functions; first-order time-independent perturbation theory for non-degenerate states, application of variation treatment and perturbation treatment to the helium atom, Born-Oppenheimer approximation.

Unit IV Quantum Mechanical Applications-II *Lecture Marks 28*

Fundamentals of Many-Electron Quantum Mechanics: Antisymmetry Principle; Hartree product, Slater determinant; Slater-Condon rules;

Hartree Fock Theory: Hartree Fock equations, Koopmans 'and Brillouin's theorems, Roothaan equations, SCF procedure.

Computational treatment of atoms and molecules: Semi-empirical and bound-state ab initio quantum mechanical and introduction to density functional theory: Hohenberg-Kohn theorems; chemical concepts within the density functional theory, understanding of basis set types and sizes, computational scalability, Hartree-Fock and Post-Hartree-Fock calculations for determining electronic energies and associated molecular properties, electronic structure and thermochemical properties, geometry optimization, study of reaction mechanism, transition-state optimizations.

Suggested Readings

- Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry, 11th Ed., Oxford University Press, New Delhi (2018).
- Kalidas, C.; Sangaranarayanan, M. V., Non-Equilibrium Thermodynamics-Principles and Applications, Macmillan Publishers India, New Delhi

- Lebon, G.; Jou, D.; Casas-Vazquez, J., Understanding Non-equilibrium Thermodynamics: Foundations, Applications, Frontiers, Springer, Heidelberg (2008). 3. Prigogine, I., Introduction to Thermodynamics of Irreversible Processes, 3rd Ed., Wiley (1968).
- Gupta, M. C., Statistical thermodynamics, New Age International Publishers, New Delhi (2007).
- Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry; 47th Ed, Vishal Publishing, New Delhi (2017).
- McQuarrie, D. A., Statistical Mechanics, Viva Books, New Delhi (2003).
- Chandra, A. K., Introductory Quantum Chemistry, 4th Ed., McGraw Hill Education India, New Delhi (2017).
- Levine, I. N., Quantum Chemistry, 7th Ed., Pearson Education India, New Delhi (2016).
- McQuarrie, D. A., Quantum Chemistry, Viva Books, New Delhi (2016).
- Jensen, F., Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell, New Jersey (2017). Further Reading
- Sen, B. K., Quantum Chemistry Including Spectroscopy, 2nd Ed., Kalyani Publishers, New Delhi (2004).
- Prasad, R. K., Quantum Chemistry, 4th Ed., New Age International Publishers, New Delhi (2010).

PG Semester III

NCrF level	*6.5*
Title of the Course	*Elective-I (Advanced Solid State Chemistry and Functional Materials)*
Course code	*CHME-301*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Understand the principles governing the synthesis, crystal growth, structural modification and characterization of inorganic solids and nanomaterials.
- Explain the relationships between structure, composition and physical properties of advanced functional materials, including semiconductors, superconductors, composites and nanostructured materials.
- Develop knowledge of modern synthetic techniques such as sol-gel, hydrothermal, combustion, chemical vapour deposition and template-assisted synthesis for preparing advanced materials.
- Correlate the electronic, optical, magnetic and surface properties of materials with their practical applications in energy, catalysis, sensing and environmental technologies.
- Understand the chemistry and applications of carbon-based materials, nanocomposites, nanoparticles, nanowires and other emerging nanostructured materials.
- Develop the ability to evaluate advanced materials for technological applications through critical analysis of their synthesis, properties and performance.

Course Outcomes (COs)

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

CO1: Explain the principles and methodologies used for the synthesis, crystal growth and modification of inorganic solids, thin films and nanostructured materials.

CO2: Describe the synthesis, structure and properties of intercalation compounds, carbon nanomaterials, semiconductor nanostructures and composite materials.

CO3: Correlate the structural, electronic, optical and surface properties of advanced materials with their chemical composition and synthesis methods.

CO4: Explain the principles of superconductivity, functional composites and advanced materials used in catalysis, energy storage, sensing and biomedical applications.

CO5: Interpret the influence of particle size, morphology, quantum confinement and surface plasmon resonance on the properties of nanoscale materials.

CO6: Evaluate modern characterization techniques used to determine crystal structure, particle size, morphology and surface properties of solid materials.

CO7: Analyse the applications of advanced materials in photovoltaics, fuel cells, photocatalysis, electrochemical devices, sensors and other emerging technologies.

CO8: Critically assess recent developments in solid-state chemistry, nanoscience and functional materials and apply these concepts to research and technological innovation.

Unit I Synthesis and Modification of Inorganic Solids *Lecture/Marks: 25*

High temperature methods; co-precipitation and precursor method, sol-gel method; combustion synthesis, intercalation/de-intercalation reactions; High pressure synthesis hydrothermal and template synthesis; chemical vapour deposition (CVD), Preparation of crystalline materials, nucleation, crystal growth

Graphite and zirconium intercalation compounds, transition metal chalcogenide, thin films, growth of single crystals.

Catalyst immobilization onto silica and clay surfaces and applications, pillaring of certain clays

Electronic and optical properties of some inorganic and organic solids (Solid electrolytes, Inorganic coloured solids, white and black pigments)

Design and properties of composites, polymer matrix and carbon-carbon composites, Synthesis of nanoparticle semiconductors, nanowires and nanorods; Synthesis, structures and properties of C60 and related compounds; Synthesis, structures and applications of single walled (SWNTs), multi-walled (MWNTs) carbon nanotubes, other synthetic methods of nanomaterials (micellar and template based methods).

Unit II Chemistry of Advanced Materials *Lecture/Marks: 20*

Superconductors: Brief history of superconductors, Properties of superconductors-critical temperature, effect of magnetic field; BCS theory; Superconductivity in 1-2-3 materials. Applications of superconducting materials, Organic superconductors, Fullerenes and doped fullerenes as superconductors, Intercalation compounds of graphite, Polymer-clay nanocomposites, Carbon-Carbon and polymer composite, Surface modification of nanomaterials with specific example to metal and metal oxide nanoparticles and their application in drug delivery, sensors, biosensors, catalysis, and in energy sector

Unit III Introduction to Physics and Chemistry of solid materials *Lecture/Marks: 25*

Conductor, semiconductor and insulator; Graphite, graphene-oxide, diamond. Size and morphology dependence properties, Methods of measuring properties: crystallography, size of particles, surface structure. Quantum confinement effect and Surface plasmon resonance. Application of various solid materials in fuel cell, photovoltaic cell, in electrochemistry as electrode materials (capacitor material), photocatalysis and chemical sensors.

Suggested books

- West, A. R., Solid State Chemistry and its Application, Wiley India, New Delhi (2007).
- Smart, L. E.; Moore, E. A., Solid State Chemistry: An Introduction, 4 th Ed., CRC Press, New Delhi (2017).
- Kakani, S. L.; Kakani, A., Material Science, 3 rd Ed., New Age International Publishers, New Delhi (2016).
- Skoog, D. A.; Holler, F. J.; Crouch, S. R., Principles of Instrumental Analysis, 6th Ed., Cengage Learning India, New Delhi (2014).
- Poole, C. P. Jr.; Owens, F. J., Introduction to Nanotechnology, Wiley India, New Delhi (2007).
- Rao, C. N. R.; Gopalakrishnan, J., New Direction in Solid State Chemistry, 2nd Ed., Cambridge University Press, Cambridge (1997).
- Keer, H. V., Principles of the Solid State, 2nd Ed., New Age International Publishers, New Delhi (2017).

PG Semester III

NCrF level	*6.5*
Title of the Course	*Elective – III (Advanced Polymer Chemistry)*
Course code	*CHME-103*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of the structure, properties, morphology and classification of polymers and their relationship to material performance.
- Understand the mechanisms, kinetics and control of various polymerization processes used in the synthesis of modern polymeric materials.
- Explain the principles and applications of molecular weight determination and advanced techniques for polymer characterization.
- Apply thermodynamic concepts to polymer solutions, polymer blends and nanocomposites for understanding their physical behaviour and stability.
- Correlate polymer structure with thermal, mechanical, rheological, electrical and functional properties.
- Appreciate the importance of advanced polymeric materials in nanotechnology, energy storage, biotechnology and sustainable materials research.

Course Outcomes (COs)

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

CO1: Classify polymers based on structure, stereochemistry and morphology, and explain the influence of molecular architecture on their physical and chemical properties.

CO2: Analyse the mechanisms, kinetics and molecular weight control of step-growth, chain-growth, ionic, coordination, ATRP, RAFT, ROMP and other advanced polymerization techniques.

CO3: Evaluate polymer molecular weight, molecular weight distribution and polymer architecture using modern analytical and spectroscopic characterization methods.

CO4: Interpret the morphology, thermal transitions and mechanical behaviour of polymers using techniques such as DSC, TGA, DMA, GPC, XRD, microscopy and rheological analysis.

CO5: Apply the principles of polymer solution thermodynamics, including Flory–Huggins theory and solubility parameters, to predict polymer–solvent interactions and phase behaviour.

CO6: Explain the preparation, characterization and performance of polymer blends, nanocomposites and functional polymeric materials.

CO7: Assess the applications of advanced polymers in nanotechnology, conducting materials, biomedical systems, energy storage and other emerging technologies.

CO8: Critically evaluate recent developments in polymer chemistry and materials science and apply polymer design principles to research and industrial applications.

Unit I: Introduction to Polymer Chemistry ***Lecture Marks 20***

Types of polymers based on their molecular structure (linear, branched, cross-linked, block) and stereochemistry of repeating units (Tacticity in polymers), chemical and geometrical structure, physical state and thermal transition: crystalline melting temperature, Tm and glass transition temperature, T_g. Properties of polymers: thermal, mechanical, rheological and electrical properties. Effect of Polymer structure on their properties. Molecular Weights and Sizes: Solubility parameters, Thermodynamics of mixing, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimm plot) Physical State and Morphology: Crystalline and Amorphous state, Thermal transitions, Glass-Rubber transition, Mechanical properties– stress-strain behavior, Elastomer, Fibers and Plastics.

Unit II: Polymerization Processes ***Lecture Marks 20***

Step polymerization, chain polymerization including carbonyl polymerization, ionic polymerization, co-ordination polymerization, atom transfer free radical polymerization, supramolecular polymerization, ring opening polymerization, metathesis polymerization, group transfer polymerization; emulsion polymerization, chain copolymerization. Reactivity ratio and control of molecular weight in polymerization.

Kinetics of polymerization, Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization. Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers. State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc.

Unit III: Polymer Characterization ***Lecture Marks 15***

Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydipersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultrantracentrifugation methods, fractionation of polymers, Gel permeation chromatography (GPC).

Chemical analysis of polymers, spectroscopic methods-IR, NMR, ESR, X-Ray Diffraction analysis; Microscopy- light Microscopy, Electron Microscopy and Electron Diffraction, Scanning electron microscopy; Thermal analysis- DSC, TGA, DMA, Rheology, Physical testing; stress-strain properties in tension Polymer Blend and Nanocomposites: Preparation, Types of blends, types of nanofillers, Thermodynamical considerations, Property enhancements

Unit IV: Thermodynamics of Polymer Solutions ***Lecture Marks 10***

Chain conformation, kinetic chain length; molecular dimensions in solution, solubility of polymers, solubility parameters, transfer process, lattice theory, thermodynamics of polymer dissolution; ΔH, ΔS and ΔG of mixing; Flory–Huggins theory, thermodynamics of dilute polymer solutions, $\chi 1$ and θ-temperature.

Unit V: Applications of Polymer ***Lecture Marks 5***

Materials and Biological importance and use. Nanomaterials, conducting polymers, Polymers for Energy applications. Physical aspects of polymers.

Suggested Reading

- *Sun, S. F., Physical Chemistry of Macromolecules: Basic Principles and Issues, 2nd Ed., Wiley-Blackwell, New York (2004).*
- *Odian, G., Principle of Polymerization, 4th Ed., Wiley-Blackwell, New York (2004).*
- *Flory, P. J., Principles of Polymer Chemistry, Asian Books, New Delhi (2006).*
- *Gowariker, V. R.; Viswanathan, N. V.; Sreedhar, J., Polymer Science, New Age International Publishers, New Delhi (2011).*
- *Misra, G. S., Introduction to Polymer Chemistry, New Age International Publishers (2008).*
- *Billmeyer, F. W., Textbook of Polymer Science, Wiley India, New Delhi (2010).*

PG Semester III

NCrF level	*6.5*
Title of the Course	*Elective – III (Molecular Rearrangements and Reactive Intermediates in Organic Synthesis)*
Course code	*CHME-302*
Paper credit	*04* (L 3 – T 1 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After completing this course, students will be able to

- Develop a comprehensive understanding of the structure, stability, generation, and reactivity of reactive intermediates in organic chemistry.
- Understand the mechanisms and synthetic applications of molecular rearrangements involving carbocations, carbanions, carbenes, nitrenes, radicals, and arynes.
- Explain the chemistry of silicon-, sulfur-, phosphorus-, boron-, and organometallic-based reagents in modern organic synthesis.
- Evaluate the role of reactive intermediates in carbon–carbon and carbon–heteroatom bond-forming reactions, stereoselective synthesis, and functional group transformations.
- Appreciate the applications of reactive intermediates and organometallic reagents in contemporary organic synthesis, medicinal chemistry, and advanced chemical research.

Course Outcomes (COs)

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

CO1: Explain the structure, stability, generation, and reactivity of reactive intermediates and correlate their properties with reaction outcomes.

CO2: Analyze the mechanisms and synthetic significance of molecular rearrangements and reactions involving carbocations, carbanions, carbenes, nitrenes, radicals, and arynes.

CO3: Apply the principles of silicon-, sulfur-, phosphorus-, boron-, and organometallic reagent chemistry in designing efficient synthetic transformations.

CO4: Evaluate reaction mechanisms, selectivity, and synthetic strategies involving reactive intermediates for complex organic synthesis.

CO5: Integrate the concepts of reactive intermediates and organometallic chemistry to solve advanced problems in synthetic organic chemistry and contemporary research.

UNIT I: Carbocations and Carbanions *(12 Hours0*

Introduction to reactive intermediates; classification; carbocations: structure, stability, generation, rearrangements; Wagner–Meerwein, Pinacol–Pinacolone, Beckmann rearrangements; carbanions: structure, stability, generation, reactivity; molecular rearrangements involving carbanions; Claisen rearrangements (Ireland-, Johnson-, Eschenmoser-, Overman-Claisen); [1,2]- and [2,3]-Wittig rearrangements; Stevens, Sommelet–Hauser, Benzilic acid, Favorskii, Neber, Smiles, Payne, Baker–Venkataraman rearrangements; Ramberg–Bäcklund reaction.

UNIT II: Carbenes and Nitrenes *(10 Hours)*

Carbenes: history; classification; structure; molecular orbital theory; singlet and triplet carbenes; persistent and metallocarbenes; generation from diazo compounds, tosylhydrazones, ketenes, strained rings, strained alkenes, and α-elimination; addition, insertion, cyclopropanation; Simmons–Smith, Bamford–Stevens, Shapiro, Wolff rearrangements; alkene metathesis; nitrenes: structure, stability, generation, reactivity, synthetic transformations; Curtius, Lossen, Schmidt rearrangements.

UNIT III: Free Radical Chemistry *(12 Hours)*

Free radicals: structure, stability, generation, ESR spectroscopy, chain reactions, abstraction, addition and elimination processes; halogenation reactions; radical addition of HBr; regiochemistry; carbon-carbon bond formation; nucleophilic and electrophilic radicals; intramolecular and intermolecular radical reactions; radical polymerization; radical rearrangements; Barton nitrite photolysis; Barton decarboxylation; Barton-McCombie deoxygenation; Hunsdiecker reaction; Birch reduction; chain walking polymerization; Norrish Type I and II reactions; Kolbe electrolysis; radical coupling; Sandmeyer reaction; applications of radical chemistry.

UNIT IV: Arynes and Benzyne Chemistry *(8 Hours)*

Structure and bonding of benzyne; comparison with benzene and acetylene; methods of aryne generation; dehydrohalogenation of aryl halides; metal–halogen exchange; anthranilic acid route; fragmentation methods; Kobayashi and Hosoya methods; cesium carbonate activation; cycloaddition, arylation, insertion, metal-catalyzed, rearrangement and multicomponent reactions involving arynes.

UNIT V: Silicon-Based Reagents in Organic Synthesis *(6 Hours))*

Nature of silicon bonding; comparison of carbon and silicon; α- and β-silicon effects; nucleophilic substitution at silicon; silyl protecting groups; TMS-OTf; TMS-CN; alkynyl-, vinyl-, and allylsilanes; hydrosilylation; Hiyama coupling; Peterson elimination; Brook rearrangement; ipso substitution; Silyl-Heck and Silyl-Negishi coupling reactions.

UNIT VI: Sulfur- and Phosphorus-Based Reagents *(10 Hours)*

Sulfur ylides; sulfur-stabilized anions; Julia olefination; electrophilic sulfur and selenium reagents; allylic sulfoxide rearrangement; Pummerer rearrangement; Swern, Corey-Kim and Kornblum oxidations; Chugaev elimination; Corey-Chaykovsky epoxidation and cyclopropanation; Mislow-Evans and Ramberg-Bäcklund rearrangements; Smith-Tietze coupling; phosphorus reagents; Appel, Mitsunobu, Arbuzov, Wittig, Horner-Wadsworth-Emmons, aza-Wittig, Corey-Fuchs, Corey-Nicolaou, Corey-Winter, Seyferth-Gilbert, Staudinger and Vilsmeier-Haack reactions.

UNIT VII: Organoboron Chemistry *(4 Hours)*

Structure and reactivity of organoboron compounds; hydroboration-oxidation; cross-coupling reactions; radical transformations; boron-mediated rearrangements; 1,2-metallate rearrangement; Matteson and Aggarwal homologations; Zweifel olefination; Boron-Wittig reaction.

UNIT VIII: Contemporary Developments in Total Synthesis *(10 Hours)*

Organolithium reagents: structure, aggregation, generation, metal–halogen exchange, transmetallation, deprotonation, lithiation, ortho-lithiation, chelation, solvent effects, aldehyde synthesis, umpolung and asymmetric synthesis; Grignard reagents: structure, preparation, mechanism and reactivity; organozinc reagents: preparation, activated zinc, Rieke zinc, transmetallation, Negishi coupling, Reformatsky and Blaise reactions, Simmons–Smith reaction; organocopper reagents: Gilman reagents, synthesis, reactivity and comparison with Grignard reagents.

Suggested readings

- Organic Chemistry 2nd Edition, by J. Clayden, S. Warren, N. Greeves, P. Worthers, Oxford University Press.
- Advanced Organic Chemistry (Part B: Reactions and synthesis) by F. A. Carey and R. J. Sundberg, 5th Corrected ed, 2008.
- Modern Methods of Organic Synthesis by William Carruthers and Ian Coldham, CambridgeUniversity Press; 4th edition, 2004.
- Organic Chemistry Vol 1 by I. L. Finar, Pearson Education India; 6th edition, 2002.

N.B. Student can take similar MOOCs course available online in NPTEL/SWAYAM

https://onlinecourses.nptel.ac.in/e-learning/preview/noc26_cy70

PG Semester III

NCrF level	*6.5*
Title of the Course	*Elective – IV (Transition Metal Organometallic Chemistry: Principles to Applications)*
Course code	*CHME-304*
Paper credit	*04 (L 4 – T 0 - P 0)*
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

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

- Develop a comprehensive understanding of the fundamental principles of organometallic chemistry, including the nature of metal–carbon bonding, classification, electronic structure, and molecular geometry of organometallic compounds.
- Understand the synthesis, characterization, electron counting methods, and structural features of organometallic compounds using modern spectroscopic and analytical techniques.
- Explain the mechanisms of fundamental organometallic reactions and apply mechanistic concepts to predict the reactivity and stability of transition metal complexes.
- Evaluate the role of organometallic compounds in homogeneous catalysis, industrial chemical processes, organic synthesis, and sustainable chemical transformations.
- Appreciate the applications of organometallic chemistry in biological systems, medicinal chemistry, and emerging areas of materials science and catalysis, thereby developing the ability to relate fundamental concepts to contemporary research.

Course Outcomes (COs)

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

CO1: Classify organometallic compounds, explain their electronic structures and bonding characteristics, and apply electron counting methods, the Effective Atomic Number (EAN) concept, and the eighteen-electron rule to predict their stability and structure.

CO2: Describe the synthesis, purification, and characterization of organometallic compounds using spectroscopic and analytical techniques such as IR, NMR, UV–Visible spectroscopy, mass spectrometry, X-ray crystallography, and magnetic measurements.

CO3: Analyze the mechanisms of fundamental organometallic reactions, including ligand substitution, oxidative addition, reductive elimination, migratory insertion, β-hydride elimination, C–H bond activation, and related transformations.

CO4: Explain the principles of homogeneous catalysis and evaluate the role of organometallic catalysts in industrial processes, cross-coupling reactions, polymerization, hydrogenation, hydroformylation, and other important catalytic transformations.

CO5: Apply the principles of organometallic chemistry to organic synthesis, bioorganometallic chemistry, medicinal chemistry, and contemporary research problems involving catalysis, sustainable chemistry, and advanced functional materials.

Unit I: Introduction to Organometallic Chemistry (5 Hours)

Definition of organometallic chemistry; historical development; scope and importance of organometallic chemistry; classification of organometallic compounds; metal–carbon σ-bonded compounds; metal–carbon π-bonded compounds; transition metal complexes; organometallic ligands; nature of metal–carbon bonding; applications in homogeneous catalysis; industrial applications; organometallic compounds in biological systems; contemporary developments in organometallic chemistry.

Unit II: Bonding in Organometallic Compounds (8 Hours)

Electronic structure of transition metals; ligand field considerations; covalent bonding model; Dewar–Chatt–Duncanson model; σ-donation; π-back donation; synergic bonding; metal–ligand interactions; carbon monoxide as ligand; metal carbonyl complexes; nitrosyl complexes; phosphine ligands; isocyanide ligands; metal–alkyl compounds; metal–aryl compounds; metal–hydride compounds; factors influencing bond strength and stability.

Unit III: Electron Counting and Structure (6 Hours)

Valence electron counting; neutral atom method; ionic method; effective atomic number (EAN); eighteen-electron rule; exceptions to the eighteen-electron rule; prediction of stability; coordination geometry; metal clusters; bridging ligands; metal–metal bonding; structural features of organometallic compounds.

Unit IV: Synthesis and Characterization of Organometallic Compounds (6 Hours)

Direct synthesis; oxidative addition; reductive elimination; salt metathesis; transmetallation; ligand substitution; carbonylation; photochemical synthesis; electrochemical synthesis; purification of organometallic compounds; infrared spectroscopy; nuclear magnetic resonance spectroscopy; ultraviolet-visible spectroscopy; mass spectrometry; X-ray crystallography; magnetic susceptibility measurements; structural characterization.

Unit V: Fundamental Organometallic Reactions (8 Hours)

Ligand substitution reactions; oxidative addition; reductive elimination; migratory insertion; carbon monoxide insertion; alkene insertion; β-hydride elimination; α-hydride elimination; nucleophilic attack on coordinated ligands; electrophilic attack on coordinated ligands; cyclometallation; C–H bond activation; σ-bond metathesis; reaction mechanisms; kinetic and thermodynamic considerations.

Unit VI: Organometallic Catalysis (7 Hours)

Principles of homogeneous catalysis; catalytic cycles; Wilkinson catalyst; Vaska's complex; hydrogenation; hydroformylation; hydrosilylation; carbonylation; olefin polymerization; Ziegler–Natta catalysts; metallocene catalysts; cross-coupling reactions; Heck reaction; Suzuki–Miyaura reaction; Negishi reaction; Sonogashira reaction; Stille reaction; industrial catalytic processes.

Unit VII: Organometallic Compounds in Organic Synthesis (3 Hours)

Organolithium compounds; Grignard reagents; organozinc compounds; organocopper compounds; organoboron compounds; carbon–carbon bond formation; carbon–heteroatom bond formation; selective functional group transformations; asymmetric synthesis; synthetic applications of organometallic reagents.

Unit VIII: Bioorganometallic and Medicinal Organometallic Chemistry (2 Hours)

Bioorganometallic chemistry; naturally occurring organometallic compounds; metalloenzymes; ferrocene derivatives; medicinal organometallic compounds; anticancer organometallic complexes; diagnostic applications; emerging therapeutic applications; recent advances in bioorganometallic chemistry.

Suggested readings

- Elschenbroich, C., *Organometallics*, 3rd Edition, Wiley-VCH, 2006.
- Crabtree, R. H., *The Organometallic Chemistry of the Transition Metals*, 7th Edition, Wiley, 2019.
- Hartwig, J. F., *Organotransition Metal Chemistry: From Bonding to Catalysis*, University Science Books, 2010.
- Collman, J. P., Hegedus, L. S., Norton, J. R., and Finke, R. G., *Principles and Applications of Organotransition Metal Chemistry*, University Science Books.
- Spessard, G. O. and Miessler, G. L., *Organometallic Chemistry*, 3rd Edition, Oxford University Press.
- Miessler, G. L., Fischer, P. J., and Tarr, D. A., *Inorganic Chemistry*, 6th Edition, Pearson.
- Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education.
- Shriver, D. F., Weller, M., Overton, T., Rourke, J., and Armstrong, F., *Shriver and Atkins' Inorganic Chemistry*, Oxford University Press.
- Cotton, F. A., Wilkinson, G., Murillo, C. A., and Bochmann, M., *Advanced Inorganic Chemistry*, 6th Edition, Wiley.
- Basolo, F. and Pearson, R. G., *Mechanisms of Inorganic Reactions*, Wiley.
- Madan, R. D., *Modern Inorganic Chemistry*, S. Chand Publishing.
- Sathya Prakash, G. D. Tuli, S. K. Basu and R. D. Madan, *Advanced Inorganic Chemistry*, S. Chand Publishing.
- Puri, Sharma and Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing.
- J. D. Lee (Indian Adaptation), *Concise Inorganic Chemistry*, Wiley India.

N.B. Student can take similar MOOCs course available online in NPTEL/SWAYAM

PG Semester III

NCrF level	*6.5*
Title of the Course	*Elective-V (Advanced Stereochemistry and Organic Reactions)*
Course code	*CHME-305*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course objectives

After successful completion of this course, students will be able to:

- Understand the conformational behavior of acyclic and cyclic organic molecules and correlate stereo-electronic effects with molecular stability and chemical reactivity.
- Explain the principles of stereoselectivity, stereochemical models and methods for determining absolute configuration in asymmetric organic reactions.
- Develop a comprehensive understanding of the strategies employed for the construction, transformation and interconversion of carbocyclic and macrocyclic ring systems.
- Correlate mechanistic pathways with stereochemical outcomes in elimination, substitution, neighboring group participation and ring-forming reactions.
- Apply the principles of organoboron, organosilicon and organotin chemistry in stereoselective synthesis, carbon–carbon bond formation and functional group transformations.
- Appreciate the significance of advanced stereochemistry and organo-main-group chemistry in modern organic synthesis, catalysis and research-oriented applications.

Course outcomes (COs)

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

CO1: Explain the conformational preferences of acyclic and cyclic systems by analysing steric, electronic and stereoelectronic effects, including A-strain, anomeric effect, transannular interactions and conformational equilibria.

CO2: Interpret the stereochemical course of elimination, substitution, neighboring group participation, esterification and epoxide formation and ring-opening reactions using established stereochemical principles and mechanistic concepts.

CO3: Analyse stereoselective organic reactions using Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk, Cieplak, cation coordination and Zimmerman-Traxler models, and determine absolute configuration by appropriate methods.

CO4: Explain the mechanistic principles involved in the synthesis, cyclization and interconversion of three-, four-, five-, six-membered and macrocyclic ring systems using classical and modern synthetic methodologies.

CO5: Apply the principles of organoboron chemistry to hydroboration, boron-mediated rearrangements, allylboration reactions, asymmetric synthesis and carbon–carbon bond-forming transformations.

CO6: Interpret the reactivity and synthetic applications of organosilicon compounds, including protecting group strategies, β-silicon effect, Peterson olefination, Brook rearrangement and stereoselective synthesis.

CO7: Analyse the preparation, reactivity and stereochemical applications of organotin compounds in radical reactions, hydrostannylation, tin-lithium exchange and carbon–carbon bond-forming processes.

CO8: Critically evaluate stereochemical and mechanistic aspects of advanced organic transformations and apply contemporary synthetic strategies involving cyclic systems and organo-main-group reagents to research-oriented problems.

Unit I Advanced stereochemistry ***Lecture Marks 20***

(a) Conformational analysis: Introduction to conformational analysis, steric, electronic and stereoelectronic effects in governing the conformation of acyclic and cyclic (5 and 6 membered rings) systems, A-strains and anomeric effect, decalins, transannular interactions in medium size rings.

b) Conformation and reactivity: steric and electronic effects in syn-elimination, E2 elimination and neighboring group participation (Woodward, Prevost methods) of acyclic and cyclohexyl systems, esterification, substitution reaction and formation and opening of epoxide in cyclohexyl systems (Furst Plattner rule).

Unit II Reaction Mechanism applying Stereochemistry ***Lecture Marks 15***

Stereoselectivity: Classification, terminology, principle of stereoselectivity, examples of diastereoselectivity using Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk models, Cieplak and cation coordination models, and Zimmerman-Traxler transition states, enantioselectivity. Desymmetrization and kinetic resolution, methods of determination of absolute configuration.

UNIT III Some special reactions on cyclic systems ***Lecture Marks 20***

Construction of Ring Systems: (a) Different approaches towards the synthesis of three, four, five, and six-membered rings. (b) Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). (c) Construction of macrocyclic rings (Intramolecular Free Radical Cyclizations: Acyloin Condensation, Pinacol Coupling, McMurry Reaction. Cation-π Cyclizations, Pericyclic Reactions) and ring closing metathesis.

Unit IV Organo-main-group chemistry ***Lecture Marks 15***

Organoboron Chemistry: Preparation and properties of organoboron compounds; hydroboration of alkenes and alkynes, hydroboration-oxidation, hydroboration of carbonyl compounds, boron-mediated rearrangements, allylboration reactions, organoboron compounds in asymmetric synthesis and C-C bond formation.

Organosilicon Chemistry: Preparation and reactions of organosilicon compounds; trimethylsilyl

(TMS) group as a protecting and activating group; β-silicon effect; allylsilanes and vinylsilanes in electrophilic substitution; Peterson olefination; Brook rearrangement; sila-Pummerer rearrangement; organosilicon compounds in stereoselective synthesis.

Organotin Chemistry: Preparation and properties of organotin compounds; tributyltin hydride in radical reactions; allyl-, vinyl- and arylstannanes in synthesis; hydrostannylation; tin-lithium exchange; stereochemical aspects and synthetic applications of organotin reagents.

Suggested Readings

- *Zweifel, G. S., Nantz, M. H., Somfai, P. Modern Organic Synthesis: An Introduction, 2nd Edn., Wiley, New York, 2017.*
- *Clayden, J., Greeves, N., & Warren, S. Organic Chemistry (3rd ed.). Oxford University Press, 2021.*
- *March, J., Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.*
- *Carey, F. A., & Sundberg, R. J. Advanced Organic Chemistry, Part B: Reactions and Synthesis (5th ed.). Springer, 2007.*

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Advanced Inorganic Chemistry -IV*
Course code	*CHMP-401*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of inorganic chains, rings, polymers and their structural diversity, bonding and applications.
- Explain the chemistry of aqueous, non-aqueous and molten salt solvents and their significance in inorganic reactions.
- Understand the principles of bioinorganic chemistry with emphasis on metal–nucleic acid interactions, oxidative stress and metal-based therapeutics.
- Develop an in-depth understanding of supramolecular chemistry, including molecular recognition, self-assembly and host–guest interactions.
- Correlate supramolecular architectures with their applications in catalysis, sensing, molecular devices, nanotechnology and biomedical sciences.
- Appreciate the role of modern inorganic chemistry in the development of functional materials, molecular machines and advanced therapeutic systems.

Course Outcomes (COs)

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

CO1: Explain the synthesis, structure, bonding and properties of inorganic chains, rings, polymers, silicates, phosphazenes, polyoxometalates and related materials.

CO2: Compare the properties and reactivity of aqueous, non-aqueous and molten salt solvents and evaluate their roles in inorganic chemical processes.

CO3: Analyse the mechanisms of metal–DNA interactions, including coordination, intercalation, insertion and photocleavage, and relate them to biological and therapeutic applications.

CO4: Explain the biochemical significance of metal complexes in oxidative stress, anticancer activity, photodynamic therapy and nanoparticle-mediated drug delivery.

CO5: Interpret the principles of supramolecular chemistry, molecular recognition and host–guest interactions involving crown ethers, cryptands, calixarenes, cyclodextrins and related systems.

CO6: Evaluate the design, synthesis and applications of self-assembled supramolecular systems, including coordination polymers, metal–organic frameworks (MOFs), catenanes, rotaxanes and molecular knots.

CO7: Explain the operation and applications of supramolecular catalysts, molecular switches, molecular machines, electronic devices and chemical sensing systems.

CO8: Critically analyse contemporary developments in inorganic materials, bioinorganic chemistry and supramolecular chemistry and apply these concepts to interdisciplinary research.

Unit I Inorganic Chains, Rings and Polymers ***Lecture/Marks: 15***

Chains: Catenation, hetero catenation, silicates, aluminosilicates, zeolites and clays, intercalation, 1-D conductors, isopoly anions, heteropolyanions

Rings: Borazene, Phosphazene polymer, heterocyclic and homocyclic inorganic rings

Types of inorganic polymers, comparison with organic polymers, Synthesis, structure and bonding in sulphur-nitrogen compounds, siloxanes, iso- and hetero-poly anions.

Unit II Chemistry of Aquous and non-aquous solvents ***Lecture/Marks: 10***

Water, ammonia, solutions of metals in ammonia, sulphuric acid, protic and aprotic solvents, Molten salt as solvent

Unit III Metal -Nucleic acid interaction ***Lecture/Marks: 15***

Various types of interactions of metal complexes with DNA– coordination, intercalation, insertion, electrostatic & H bonding. Interaction of tris(phenanthroline) Ru complex with DNA & monitoring techniques. Applications of metal complex nucleic acid interactions. Interactions of cis-platin with DNA – evidence, kinetics, crosslinking reactions, biological consequences. Photodynamic therapy-photocleavage of DNA by transition metal (Fe and Ru) complexes and its therapeutic implications. Oxidative stress due to iron and copper via Fenton mechanism and its consequences in human diseases. Inorganic nanoparticle in drug delivery.

Unit IV Supramolecular Chemistry ***Lecture/Marks: 25***

Introduction to Supramolecular Chemistry: Definition of Supramolecular Chemistry, Biological Inspiration for Supramolecular Chemistry, Non-covalent interactions, Host-Guest interactions, Pre-organisation: Kinetic and Dynamic Effects, and complimentarity, lock and key analogy.

Synthesis, structure and their applications in recognitions: Crown ethers, podands, lariat ethers, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands binding of organic and inorganic cationic, anionic, ion pair and neutral guest molecules with host molecules, Supramolecular chiral recognition, ion-transport in biological system.

Self-Assembly of molecules: Design, synthesis and applications of metallomacrocycles, coordination polymers like Metal Organic Frameworks (MOFs), catenanes, rotaxanes, helicates and knots. Biochemical self-assembly. Surfactants, Micelles and Vesicles, Supramolecular Liquid Crystals.

Supramolecular Catalysis: Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, Corands as ATPase Mimics, abiotic supramolecular catalysis.

Molecular Devices: Philosophy of molecular devices, Molecular and supramolecular photonic devices, Light conversion and energy transfer devices, Molecular and supramolecular electronic devices, Molecular wires, rectifiers, Molecular switches (Photo, electro, mechano, etc.), Molecular machines (gear, break, paddle wheel, shuttle etc.), Molecular and supramolecular electrochemical devices, supramolecular semiochemistry and sensing, Logic gates.

Suggested Reading

- F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann – Advanced Inorganic Chemistry
- D. F. Shriver and P. W. Atkins – Shriver and Atkins' Inorganic Chemistry
- Gary L. Miessler, Paul J. Fischer and Donald A. Tarr – Inorganic Chemistry
- J. E. Huheey, E. A. Keiter and R. L. Keiter – Inorganic Chemistry: Principles of Structure and Reactivity
- J. D. Lee – Concise Inorganic Chemistry
- Jonathan W. Steed and Jerry L. Atwood – Supramolecular Chemistry
- Jean-Marie Lehn – Supramolecular Chemistry: Concepts and Perspectives
- Fritz Vögtle – Supramolecular Chemistry: An Introduction
- Stephen J. Lippard and Jeremy M. Berg – Principles of Bioinorganic Chemistry
- Ivano Bertini, Harry B. Gray, Stephen J. Lippard and Joan Selverstone Valentine – Bioinorganic Chemistry
- K. Nakamoto – Infrared and Raman Spectra of Inorganic and Coordination Compounds
- C. N. R. Rao and J. Gopalakrishnan – New Directions in Solid State Chemistry
- Anthony R. West – Solid State Chemistry and Its Applications
- Harry B. Gray and John M. Berg – Bioinorganic Chemistry
- P. D. Beer, P. A. Gale and D. K. Smith – Supramolecular Chemistry

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Advanced Organic Chemistry - IV*
Course code	*CHMP-402*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course objectives

After successful completion of this course, students will be able to:

- Understand the principles and applications of modern spectroscopic techniques for the structural elucidation of organic molecules.
- Explain the structural, stereochemical and biological aspects of carbohydrates, amino acids, peptides, proteins and nucleic acids.
- Develop a comprehensive understanding of the chemistry, biosynthesis and biological significance of natural products, including terpenoids, alkaloids and steroids.
- Correlate spectroscopic data with molecular structure, stereochemistry, conformation and reaction pathways in organic compounds.
- Apply spectroscopic methods and biomolecular concepts to solve structural and mechanistic problems in organic chemistry.
- Appreciate the significance of advanced spectroscopic techniques and bioorganic molecules in chemical, biological, medicinal and pharmaceutical research.

Course outcomes (COs)

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

CO1: Explain the principles of NMR and mass spectrometry, and interpret spectroscopic parameters for the structural characterization of organic compounds.

CO2: Analyse one- and two-dimensional NMR spectra, including ^{1}H, ^{13}C, DEPT, COSY, HMQC, HSQC and NOE techniques, for the elucidation of molecular structure, stereochemistry and dynamic processes.

CO3: Interpret mass spectral fragmentation patterns, isotope abundance, high-resolution and soft ionization mass spectrometric data, and integrate IR, NMR and mass spectral information for comprehensive structure elucidation.

CO4: Explain the structure, stereochemistry, conformational behaviour, reactions and biological significance of carbohydrates, including monosaccharides, disaccharides and polysaccharides.

CO5: Analyse the chemistry of amino acids, peptides, proteins and nucleic acids by correlating their structures, synthesis, sequencing, biosynthesis and biological functions with molecular properties.

CO6: Interpret the occurrence, biosynthesis, stereochemistry, structure elucidation and synthetic approaches of representative terpenoids, and correlate their structural features with chemical reactivity and biological activity.

CO7: Explain the classification, isolation, structure elucidation, biosynthesis and synthesis of representative alkaloids and steroids, and evaluate their biological and physiological significance.

CO8: Critically evaluate spectroscopic, structural and biosynthetic information for bioorganic molecules and natural products, and apply advanced concepts of organic chemistry to research-oriented and interdisciplinary problems.

Unit I Analysis of organic compounds via NMR and Mass	*Lecture Marks 25*

(a) NMR Spectroscopy: NMR phenomenon, spin ½ nuclei, (^{1}H, ^{13}C, ^{31}P and ^{19}F), ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Second order effects, examples of AB, AX, AA'BB' and ABX systems, simplification of second order spectrum, application of NMR data for stereochemical assignments, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation of nuclear spins, NOE effects, ^{1}H and ^{13}C chemical shifts to structure correlations. Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion.

(b) Application of DEPT technique to the analysis of CH multiplicities in ^{13}C NMR spectroscopy. Correlation spectroscopy: Illustration of practical applications of ^{1}H-^{1}H COSY, ^{1}H-^{13}C COSY, NOE difference spectroscopy (stereochemistry determination), HMQC and HSQC techniques.

(c) Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, basic principle of ionization and ion analysis, illustrative examples from simple organic molecules to macromolecules and supramolecules. Structure elucidation problems using the above spectroscopic techniques.

(d) Applications of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds.

UNIT II Carbohydrates	*Lecture Marks 10*

Monosaccharides, Aldoses up to 6 carbons, structure of D-glucose & D- fructose (configuration & conformation), anomeric effect, mutarotation, Important reactions and conversions including protection/deprotection protocol, Disaccharides and polysaccharide: nature of glycosidic linkages. Structure, reaction and conformation of disaccharides – sucrose, maltose and lactose. Polysaccharides – starch and cellulose.

Unit III Amino acids	*Lecture Marks 10*

Structure of amino acids and physical and chemical properties, method of synthesis (including Merrifield synthesis) of peptides and polypeptides, naming of polypeptides chain, amino acid sequence determination (N-terminal and C terminal), structure of protein (Helical and pleated structure), denaturation of protein, biosynthesis of proteins, therapeutic and diagnostic applications.

Unit III Amino acids	*Lecture Marks 10*

Structure of purines and pyrimidine bases and their biosynthesis, nucleosides and nucleotides and their nomenclature, structure of RNA and DNA, replication of DNA and mutagenesis, codon, anticodon, t-RNA, structure and genetic code, transcription and translation.

Unit IV Terpenoids, Alkaloids and steroids — *Lecture Marks 15*

Occurrence, classification, nomenclature and isoprene rule; general methods of isolation; biosynthesis of mono- and sesquiterpenes; structure elucidation by chemical and spectroscopic methods; stereochemistry and retrosynthetic approach. Structure and synthesis of representative terpenoids: Acyclic-Linalool; Monocyclic-Terpineol, Menthol; Bicyclic-α-Pinene, Camphor, Borneol.

Alkaloids: Occurance, classification, general methods of isolation, test for detection. Structure elucidation by physical and chemical methods and synthesis (including retrosynthetic approach) of: Piperine, Papaverine, Atropine and Morphine.

Introduction, classification and biological significance; sterols: structure, stereochemistry and biosynthesis; cholesterol: constitution, conformation and biological functions; bile acids: isolation, constitution, biosynthesis and physiological functions; steroid hormones: classification, biosynthesis, biological significance, constitution and synthesis of oestrone and androsterone.

Suggested Readings

- *Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., Spectrometric Identification of Organic Compounds, 8th Ed., Wiley India, New Delhi (2015).*
- *Kemp, W., Organic Spectroscopy, 3rd Ed., Macmillan Publishers India, New Delhi (2011).*
- *Gunther, H., NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 2nd Ed., Wiley India, New Delhi (2010).*
- *Bruice, P. Y. Organic Chemistry (8th ed.). Pearson Education, 2016.*
- *Berg, J. M.; Tymoczko, J. L.; Gatto Jr., G. J.; Stryer, L., Biochemistry, 9th Ed., W. H. Freeman, New York (2019).*
- *Voet, D.; Voet, J. G., Pratt, C. W., Biochemistry, 4th Ed., John Wiley and Sons, New Jersey (2012).*
- *Campbell, M. K.; Farrell, S. O., Biochemistry, 8th Ed., Brooks/Cole, Belmont (2015).*
- *Nelson, D. L.; Cox, M. M., Lehninger Principles of Biochemistry, 7th Ed., W. H. Freeman, New York (2017).*

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Advanced Physical Chemistry - IV*
Course code	*CHMP-403*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of advanced experimental techniques used for investigating fast chemical reactions and reaction dynamics.
- Explain the kinetic behaviour of reactions in solution and the influence of molecular interactions, solvent properties and transport phenomena on reaction rates.
- Understand molecular reaction dynamics, potential energy surfaces and modern theories describing unimolecular and ultrafast chemical reactions.
- Apply advanced statistical mechanical concepts to describe liquids, phase transitions and molecular systems.
- Develop proficiency in computational approaches such as Monte Carlo and Molecular Dynamics simulations for studying chemical systems.
- Correlate theoretical models with experimental observations in chemical kinetics, reaction dynamics and statistical mechanics.

Course Outcomes (COs)

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

CO1: Explain the principles, instrumentation and applications of modern techniques for studying fast chemical reactions, including stopped-flow, relaxation methods, molecular beam experiments, NMR kinetics and shock-tube techniques.

CO2: Analyse reaction kinetics in solution by evaluating solvent effects, pressure effects, diffusion-controlled processes, electron transfer reactions and transport phenomena.

CO3: Apply linear free-energy relationships, including Hammett and Taft equations, to interpret reaction mechanisms and substituent effects.

CO4: Interpret molecular reaction dynamics using potential energy surfaces, collision theory and trajectory calculations, and explain the kinetics of unimolecular reactions using RRK and RRKM theories.

CO5: Explain the principles of femtochemistry and evaluate ultrafast molecular processes involved in chemical reactivity.

CO6: Apply advanced statistical mechanical concepts, including configurational partition functions, pair correlation functions, radial distribution functions and virial equations, to describe the properties of liquids.

CO7: Analyse phase transitions using lattice models, the Ising model, mean field theory and renormalization group concepts.

Unit I Study of Chemical Reactions *Lecture Marks 16*

Methods of studying chemical reactions: molecular beam study; stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics. Relaxation kinetics: linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time and rate constant.

Unit II Reactions in Solutions *Lecture Marks 17*

Kinetics of ion – ion and ion – dipole reactions, effect of dielectric constant on reaction rate; effect of pressure on reaction rate; cage reactions, cluster reactions, electron transfer reactions, kinetics of diffusion controlled reactions; transport phenomena; Linear free energy relationship, Hammet equation, Taft equation and their applications.

Unit III Reactions in Solutions *Lecture Marks 17*

Molecular Reaction Dynamics Potential energy surfaces; features of potential energy surfaces; estimation of activation energy and calculation of potential energy surfaces; collisions of real molecules; trajectory calculations. Dynamics of unimolecular reactions: limitations of Lindemann and Hinshelwood theory, RRK theory, RRKM theory (quantitative treatment). Femtochemistry: dynamics and chemical reactivity.

Unit III Advanced Statistical Mechanics *Lecture Marks 20*

Classical Liquids Interparticle potentials, Configurational Partition functions, distributions, pair correlation function,radial distribution function, neutron scattering experiments, Virial equation, Meyer cluster diagrams. Phase Transitions in Lattice models Lattice gas, Ising Model, order parameter, Mean Field theory, Renormalization group theory. Computer Simulations Ensemble averages, ergodicity, random numbers, Monte Carlo methods, Molecular Dynamics, constant temperature MD.

Suggested Reading

- Laidler, K. J., Chemical Kinetics, 3rd Ed., Pearson Education, New Delhi (2011).
- Rajaram, V.; Kuriakose, J. C., Kinetics and Mechanism of Chemical Transformation, McMillan India, New Delhi (2009).
- Rohatgi-Mukherjee, K. K., Fundamentals of Photochemistry, 3rd Ed., New Age International Publishers, New Delhi (2013).
- Pilling, M. J.; Pilling, S.; Seakins, P. W., Reaction Kinetics, Oxford University Press, London (1996).

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Elective VI* (Advanced Catalysis and Catalytic Materials)
Course code	*CHME-401*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of the synthesis, preparation, activation and characterization of homogeneous and heterogeneous catalysts.
- Explain the structural features, synthesis and catalytic properties of zeolites, mesoporous materials, clays and other advanced catalytic materials.
- Understand catalyst deactivation mechanisms, regeneration strategies and the design principles of catalytic reactors for industrial applications.
- Correlate catalyst composition, surface properties and pore architecture with catalytic activity, selectivity and stability.
- Explain the role of catalysis in sustainable energy production, petroleum refining, environmental protection and green chemical processes.
- Appreciate recent advances in catalytic science for industrial, environmental and energy-related applications.

Course Outcomes (COs)

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

CO1: Explain the principles and methodologies for the preparation, activation and characterization of bulk, supported and nanostructured catalysts.

CO2: Analyse the synthesis, structure, modification and catalytic behaviour of zeolites, mesoporous materials, pillared clays and related porous solids.

CO3: Correlate catalyst composition, support materials and surface properties with catalytic performance in heterogeneous catalytic processes.

CO4: Evaluate catalyst deactivation mechanisms, poisoning, sintering, coke formation and regeneration techniques employed in industrial catalysis.

CO5: Explain the principles of catalytic reactor design and assess the influence of heat and mass transfer on catalytic efficiency.

CO6: Analyse the catalytic processes involved in petroleum refining, hydrogen production, fuel processing, carbon dioxide utilization and chemical manufacturing.

CO7: Evaluate the applications of catalysis in energy conversion, photocatalysis, fuel cells, pollution control and environmentally sustainable technologies.

Unit I Catalysts synthesis and preparation *Lecture/Marks: 20*

Catalyst preparation methods – precipitation and co-precipitation – sol gel process–Dispersed metal catalysts; support materials; preparation and structure of supports; surface properties – preparation of catalysts – interaction of metal compound with substrate surface – metal distribution within catalyst pellets – metal cluster compounds as active precursors – pre-activation treatment – drying and calcinations – activation process. Bulk catalysts and supports. Heteropoly compounds – Solid superacids.carbon as catalyst support – carbon as catalyst. Catalyst manufacture– scope and goals – catalysts prepared by precipitation – solution and slurry transfer – filtration – drying: calcining; ion exchange; extrusion; crushing and screening to produce granules; coating etc.

Unit II Zeolites, mesoporous materials and clays *Lecture/Marks: 20*

Synthesis of aluminosilicate zeolites and related silica based materials – structure, composition, zeolite synthesis, mechanism and chemistry–zeolites obtained from various reaction systems – synthesis of some selected important zeolites – titanosilicates – activation of zeolites. Modification of zeolites – ion exchange – metals supported on zeolites– dealumination and desilication of zeolites; Shape selective catalysis in zeolites. Pillared clays– properties of pillared clays.Use of coordination and organometallic compounds as pillaring.pillaring of acid activated clays Mesoporous materials - ordered mesoporous materials –synthesis of silica molecular sieve materials - characterization of mesoporous molecular sieves – catalytic properties of mesoporous materials Catalytic applications of zeolite, clays and mesoporous materials.

Unit III Catalytic reactors, deactivation of catalysts *Lecture/Marks: 15*

Deactivation of catalysts – classification of catalyst deactivation processes; general aspects of catalyst deactivation – poisoning of catalysts, poisoning of metallic catalysts, poisoning of non-metallic catalysts – poisoning of bifunctional catalysts – coke formation on catalysts – metal deposition on catalysts – sintering of catalysts; Regeneration of deactivated catalysts. Design of catalytic reactors. Mass flow and heat flow minimisation.

Unit IV Energy and catalysis *Lecture/Marks: 15*

Energy related catalysis – Perspectives in oil refining – Steam reforming – Water gas shift– Methanol synthesis – CO and CO2 hydrogenation – Methanol to hydrocarbons – Hydrotreating reactions – Catalytic reforming – Catalytic cracking, Hydrocracking. Aromatization of light alkanes, Catalytic coal gasification, Catalysis in coal liquefaction; Fuel cells – Heterogeneous photocatalysis Alkylationof aromatics: Isomerization and trans-isomerization – Dehydrogenation reactions – Hydrogenation reactions – Hydroformylation – Selective oxidations. Control of pollution from automobile exhaust-catalytic conveters, abatement of nitrogen oxides and odours.

Suggested Reading

- G. Ertl, H. Knozinger, J. Weitkamp (Eds), Preparation of Solid Catalysts, WileyVCHVerlag, 1999.
- J.R. Anderson, M. Boudart (Eds), Catalysis, Science and Technology, Vol 6, Springer-Verlag, 1984.
- J. Weitkamp and L. Puppe (Eds), Catalysis and zeolites – fundamentals and applications, Springer-Verlag, 1999.
- A. Gil, L.M. Gandia, M.A. Vincente, Catalysis Reviews Science and Engineering, 42 (2000) 145-212.
- R. Hughes, Deactivation of catalysts, Academic press, 1984. G. Ertl, H. Knozinger, J. Weitkamp, Handbook of Heterogeneous Catalysis,Vol 4 and 5, Wiley-VCH, 1997.
- R. J. Farrauto, C.H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Blackie Academic, Chapman and Hall, 1997.
- R. Pearce, W.R. Patterson, Catalysis and Chemical processes, Academic press, 1981.

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Elective VII (Advanced Environmental Chemistry)*
Course code	*CHME-402*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of atmospheric, aquatic and soil chemistry, and the chemical processes responsible for environmental pollution.
- Explain the sources, fate, transport and environmental impacts of pollutants, including greenhouse gases, aerosols, pesticides, heavy metals and hazardous wastes.
- Understand the principles of environmental toxicology, pollutant degradation and modern remediation technologies for contaminated ecosystems.
- Apply the principles of green chemistry and sustainability to minimize waste, improve resource efficiency and develop environmentally benign chemical processes.
- Evaluate green synthetic methodologies, alternative reaction media and energy-efficient technologies for sustainable chemical synthesis.
- Appreciate the role of chemistry in addressing global environmental challenges, climate change and sustainable development.

Course Outcomes (COs)

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

CO1: Explain the chemical processes occurring in the atmosphere, including ozone depletion, smog formation, aerosol chemistry, acid rain and climate change.

CO2: Analyse the sources, transport, transformation and environmental impacts of air, water and soil pollutants, and evaluate appropriate pollution control strategies.

CO3: Describe the principles of environmental toxicology, pollutant degradation, bioremediation and chemical remediation for contaminated environments.

CO4: Apply the principles and metrics of green chemistry to design environmentally sustainable chemical processes and products.

CO5: Evaluate the utilization of renewable feedstocks, biomass, carbon dioxide and catalytic systems in sustainable chemical synthesis.

CO6: Explain the mechanisms and advantages of microwave-assisted, ultrasound-assisted and solvent-free synthetic methodologies as green alternatives to conventional reactions.

CO7: Assess the role of green reagents, environmentally benign catalysts and sustainable technologies in minimizing hazardous waste and improving chemical efficiency.

Unit I Atmospheric Chemistry — *Lecture Marks 15*

Temperature and pressure variation in the atmosphere, role of free radicals in atmospheric chemistry. Catalytic processes of ozone destruction, formation of Antarctic and Arctic ozone holes. Chemistry of smog formation, VOCs and their oxidation. Acid rain. PAHs and heavy metals in aerosols, lifetime and transport of aerosol particle. Global warming and greenhouse effect, Climate change Protocols. Sources of Indoor air pollution

Unit II Water and Soil Pollution *Lecture Marks 15*

Water and Soil Pollution Sources of water pollution: agricultural and pesticidal pollutants, industrial and domestic effluent. Marine pollution, oil spills and oil pollution. Community wastewater treatment chemistry, biological process for removal of phosphorus and nitrogen from wastewater sources. Soil formation: Physical and Chemical weathering, Soil properties: Soil Texture, Cation exchange capacity, Causes of soil pollution, Chemistry and management of municipal and biomedical waste.

Unit III Environmental Toxicology and Detoxification *Lecture Marks 15*

Mechanism Organic biocides, chemical stability, photolytic and non-photolytic reactions, hydrolysis, oxidation and reduction reactions, rates of degradative reactions, mobility of biocides. Principles of toxicology, chemical solution to environmental problems, better biodegradability. Kinetics of decomposition, solid remediation, chemical remediation and bioremediation.

Unit IV Principles and Applications of Green Chemistry *Lecture Marks 25*

The Essentials of Green Chemistry: Introduction to Interdisciplinary Study of Green Chemistry, Definition of Green Chemistry

Applying the 12 Principles of Green Chemistry; Green Chemistry Metrics

Waste: production, problems and prevention

Catalysis and green chemistry; Green Chemistry and Sustainability; Green Chemistry to Health and Environment: Inherent Hazards, Challenges; Water oxidation; Conversion of CO2, Utilising CO2 as reactant.

Feedstock chemicals, Chemicals from Biomass, Concept of platform molecules‘: Conversion of biomass to value-added products. Adverse Effects of Chemicals on Health and the Environment; Green Chemistry Problems.

Real World Solutions: Designing for Materials and Energy Efficiency; Designing for Degradation. Introduction to Sustainability; Aspects of Sustainability Ethics; Designing Sustainable Solutions.

Green synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate, paracetamol, ibuprofen.

Microwave assisted reactions: Microwave assisted reactions in water (oxidation of toluene to benzoic acid, oxidation of alcohols); microwave assisted reactions in organic solvents (Diels-Alder reaction and Decarboxylation); Microwave assisted solvent-free reactions (solid state reaction)- Michael addition and Knoevenagel reaction)

Ultrasound assisted reactions: Grignard reaction, Ulmann coupling and Cannizzaro reaction under sonication.

Dimethyl carbonate (DMC), Tetrabutylammoniumtribromide (TBATB) and Rongalite as green reagents in organic synthesis. Oxidation reagents and catalysts; Biomimetic multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions. Cocrystal Controlled Solid-State Synthesis (C^3S^3)

Suggested Reading

- VanLoon G. W.; Duffey S. J., Environmental Chemistry: A Global Perspective, 4th Ed., Oxford University Press, Oxford (2017).
- Anastas, P. T.; Warner, J. C., Green Chemistry: Theory and Practice, Oxford University Press, Oxford (2005).
- Pani, B., A Textbook of Environmental Chemistry, IK International Publishing House, New Delhi (2007).
- Ahluwalia, V. K.; Kidwai M., New Trends in Green Chemistry, Springer Inida, New Delhi (2012).
- Biswas, T. D.; Mukherjee, S. K. Text Book of Soil Science, Tata McGraw Hill India, New Delhi (2017).

PG Semester IV

NCrF level	*6.5*
Title of the Course	*Elective VIII (*Nanoscience and Nanomaterials)
Course code	*CHME-403*
Paper credit	*04* (L 4 – T 0 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After successful completion of this course, students will be able to:

- Develop a comprehensive understanding of the fundamental concepts, classification and unique physicochemical properties of nanomaterials.
- Explain the principles, advantages and limitations of various top-down and bottom-up approaches for the synthesis of nanomaterials.
- Understand the operating principles and applications of advanced characterization techniques used for nanomaterials.
- Correlate the structure, morphology and surface properties of nanomaterials with their physical, chemical and functional behaviour.
- Evaluate the role of surface engineering, stabilization and functionalization in enhancing the performance of nanomaterials.
- Appreciate the applications of nanomaterials in catalysis, energy, environmental remediation, sensing and advanced technologies.

Course Outcomes (COs)

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

CO1: Explain the historical development, classification, synthesis principles and unique physicochemical properties of nanomaterials.

CO2: Analyse the structure, properties and applications of carbon nanomaterials, including fullerenes, single-walled carbon nanotubes (SWNTs) and multi-walled carbon nanotubes (MWNTs).

CO3: Evaluate various top-down and bottom-up synthetic approaches, including sol-gel, hydrothermal, vapour deposition, co-precipitation, template-assisted and green synthesis methods for nanomaterial preparation.

CO4: Interpret structural, morphological and surface characteristics of nanomaterials using advanced analytical techniques such as XRD, SEM, TEM, AFM, XPS and BET analysis.

CO5: Explain the principles and applications of ICP-MS, ICP-AES and ICP-OES for the elemental analysis and characterization of nanomaterials.

CO6: Correlate nanostructure, particle size, morphology and surface modification with the optical, electrical, magnetic and catalytic properties of nanomaterials.

CO7: Assess the importance of nanomaterial assembly, stabilization and surface functionalization for enhancing performance in technological applications.

CO8: Critically evaluate the applications of nanomaterials in catalysis, energy storage and conversion, sensors, solar cells, water purification and other emerging nanotechnologies.

Unit I Introduction to Nanomaterials ***Lecture Marks 15***

History of Nanoscience, Classification of Nanomaterials, Major challenges in nanoscience and technology.

Properties of Nanomaterials: Physicochemical properties; optical properties of nanomaterials, electrical and electronic properties; magnetic properties of nanomaterials.

Structure and properties of C60; Structure and applications of single-walled (SWNTs) and multi-walled (MWNTs) carbon nanotubes.

Unit II Synthetic Approach to Nanomaterials *Lecture Marks 20*

A brief overview of different synthesis approaches (top-down and bottom-up), thermodynamics of formation of nanomaterials.

Synthesis of nanomaterials by Vapour deposition, Precipitation and co-precipitation methods, Sol-gel methods, Hydrothermal and solvothermal methods, Micellar/ Template based synthesis, Green chemical methods

Unit III Characterization Methods of Nanomaterials *Lecture Marks 20*

X-ray methods: Introduction, basic principles, instrumentation and applications of Powder X-ray diffractometry.

Microscopy: Introduction, basic principles, instrumentation and applications of scanning electron microscopy (SEM), transmission electron microscopy (TEM), and atomic force microscopy (AFM).

Surface characterisation techniques: Introduction, basic principles, instrumentation and applications of X-ray photoelectron spectroscopy (XPS), and Brunauer-Emmett-Teller (BET) surface area analysis.

Optical spectroscopy: Introduction, basic principles, instrumentation and applications of Inductively Coupled Plasma-Mass Spectroscopy (ICP-MS), Inductively Coupled Plasma-Atomic Emission Spectroscopy (ICP-AES), and Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES).

Unit IV Applications of Nanomaterials *Lecture Marks 20*

Assembly of nanostructures and their importance for various applications. Stabilisation of nanomaterials and their importance. Surface modification of nanomaterials with specific examples of metal oxide nanoparticles and their significance. Applications of nanomaterials in sensors, batteries, solar cells, catalysis, water treatment, etc.

Suggested Reading

- Poole, C. P. Jr.; Owens, F. J., Introduction to Nanotechnology, Wiley India, New Delhi (2007).
- Pradeep, T., Nano: The Essentials-Understanding Nanoscience & Nanotechnology, Tata McGraw Hill India, New Delhi (2017).
- Braun, R. D.; Introduction to Instrumental Analysis, 2nd Ed., BSP Books, Hyderabad (2012).
- Hornyak, G. L.; Tibbals, H. F.; Dutta, J.; Moore, J. J., Introduction to Nanoscience and Nanotechnology, CRC Press, Boca Raton (2008).
- Viswanathan, B., Nanomaterials, Narosa Publishing House, New Delhi (2014).

PG Semester IV

NCrF level	*6.0*
Title of the Course	*Elective – IX (Classics in Total Synthesis)*
Course code	*CHME-405*
Paper credit	*04* (L 3 – T 1 - P 0)
Total Contact Hours	*70 hours*
Distribution of Marks	*100 (End semester examination 70 + internal assessment 30)*

Course Objectives

After completing this course, students will be able to

- Develop a comprehensive understanding of the principles and strategies of total synthesis of structurally diverse natural products.
- Understand retrosynthetic analysis, synthetic planning, and stereochemical aspects involved in complex molecule synthesis.
- Explain the mechanisms and synthetic methodologies employed in the construction of biologically important natural products.
- Evaluate the application of modern synthetic approaches in natural product synthesis, medicinal chemistry, and drug discovery.
- Appreciate recent advances in total synthesis and their significance in contemporary organic chemistry research.

Course Outcomes (COs)

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

CO1: Explain the principles of total synthesis, retrosynthetic analysis, and synthetic planning for complex natural products.

CO2: Analyze the synthetic strategies and mechanistic aspects involved in the total synthesis of carbocyclic, heterocyclic, alkaloid, steroidal, terpene, and macrocyclic natural products.

CO3: Apply stereochemical principles, functional group transformations, and modern synthetic methodologies in designing efficient synthetic routes.

CO4: Evaluate alternative synthetic approaches for biologically active natural products based on efficiency, selectivity, and strategic bond construction.

CO5: Correlate total synthesis with contemporary applications in medicinal chemistry, drug discovery, and advanced organic synthesis.

UNIT I: Introduction to Total Synthesis and Three-membered Natural Products (10 Hours)

Introduction to total synthesis; retrosynthetic analysis; synthetic planning; strategic bond disconnections; functional group interconversions; stereochemical considerations; protecting group strategies; convergent and linear synthesis; total syntheses of Illudin M; Illudin C; FR900848.

UNIT II: Four-membered and Five-membered Natural Products (8 Hours)

Synthetic strategies for strained and five-membered ring systems; total syntheses of Cubane; Endiandric Acids; Prostaglandins; Penicillin; Biotin; Lactacystin; Thienamycin.

UNIT III: Triquinanes and Polycyclic Natural Products (8 Hours)

Concept of triquinane frameworks; stereochemical construction of fused polycyclic systems; total syntheses of Isocomene; Hirsutene; Capnellene; Silphiperfolene; Silphipherfol-6-en-5-one; Modephene; Ceratopicanol; Subergorgic Acid; Deoxymagellaninone; Coriolin.

UNIT IV: Six-membered Natural Products (8 Hours)

Synthetic strategies for six-membered carbocyclic natural products; total syntheses of Longifolene; Carpanone; Mevinolin; Gibberellic Acid.

UNIT V: Total Synthesis of Alkaloids (10 Hours)

General strategies in alkaloid synthesis; stereochemical control; total syntheses of Perhydrohistrionicotoxin; Strychnine; Reserpine; Yohimbine; Quinine; Dendrobine; Morphine; Methylhomosecodaphniphyllate; Secodaphniphyllane; Lysergic Acid; Galanthamine; Epibatidine; Swainsonine; Staurosporine; Manzamine; Colchicine.

UNIT VI: Total Synthesis of Steroids and Terpenoids (8 Hours)

Synthetic approaches to steroidal and terpene natural products; total syntheses of Progesterone; Estrone; representative Steroids; Taxol; Eleutherobin; Phorbol; Periplanone; Discodermolide.

UNIT VII: Total Synthesis of Macrocyclic Natural Products (8 Hours)

Strategies for macrocyclization; macrolide synthesis; ring-closing methodologies; total syntheses of Epothilones; Zaragozic Acid C; Vineomycinone B2.

UNIT VIII: Contemporary Developments in Total Synthesis (10 Hours)

Modern approaches in total synthesis; asymmetric synthesis; catalytic and biomimetic strategies; protecting-group-free synthesis; step economy; green synthetic methodologies; recent advances and applications of total synthesis in medicinal chemistry, chemical biology, and drug discovery.

Suggested readings

- Nicolaou, K. C.; Sorensen, E. J. *Classics in Total Synthesis: Targets, Strategies, Methods*; VCH: Weinheim, 1996.
- Corey, E. J., & Cheng, X.-M. (1995). The logic of chemical synthesis. John Wiley & Sons.
- Warren, S., & Wyatt, P. (2009). Organic synthesis: The disconnection approach (2nd ed.). John Wiley & Sons
- Kurti, L.; Czako, B. Strategic Applications of Named Reactions in Organic Synthesis; Elsevier Academic Press: Amsterdam, 2005.

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