Savitribai Phule Pune University, Pune

(Formerly University of Pune)

New Syllabus of

Ph.D. Course Work in Chemistry

To be implemented with effect from Academic Year 2025-2026

Board of Studies in Chemistry

Savitribai Phule Pune University, Pune

Course List for Ph.D. course work in Chemistry

Sr. No.	Name of the Course	Credits	No. of Hours
1	**Research Methodology**	04	60
2	**Two Subject specific advanced level courses** ***Select two courses from the following:*** **Course 1: Physical Chemistry** **Course 2: Inorganic Chemistry** **Course 3: Organic Chemistry** **Course 4: Material Chemistry** **Course 5: Advanced techniques in Analytical chemistry** **Course 6: Green Chemistry** **Course 7: Drug design and development**	08	120

Research Methodology

Credits: 04 (60 Hours)

Course Outcomes

CO1: Recall the fundamental concepts, objectives, and ethical principles of scientific research, including types of research, plagiarism, and intellectual property rights.

CO2: Explain different sources of scientific literature, search databases, and types of research publications along with their structural components and ethical standards. *(Covers Units 2 & 3)*

CO3: Apply appropriate search strategies, referencing methods, and plagiarism-checking tools to identify research gaps and develop research hypotheses.

CO4: Analyze chemical data using statistical and computational tools and interpret results through graphical and numerical analysis.

CO5: Evaluate research quality using journal and author metrics, statistical validation, and ethical guidelines to ensure reliability and scientific integrity.

CO6: Design and develop a complete research proposal or publication by integrating hypothesis formulation, data interpretation, budgeting, and effective presentation skills.

Content

Unit 1: Introduction to Research (10 hrs)

Meaning & Objectives of Research, Scientific Method and Types of Research: Fundamental (Basic) vs. Applied, Qualitative vs. Quantitative, Experimental vs. Theoretical/Computational,Research Process & Problem Identification: Literature survey, hypothesis formulation, research gaps, Ethics in Research: Plagiarism, authorship, data fabrication, misconduct (case studies), Intellectual Property Rights (IPR) & Patents: Basics of patents, copyrights, trademarks

Unit 2: Literature Review and Research Ethics (8 hrs)

Scientific Literature Sources: Primary, secondary, tertiary (journals, books, patents, databases),Search Strategies & Databases: SciFinder, Reaxys, Web of Science, Scopus, Google Scholar, Research ethics: plagiarism issues, tools (Turnitin, iThenticate, etc.)

Unit 3: Types of Articles and Research Metrics (12 hrs)

Types of Technical Documents: full-length papers, short communications, letters, reviews, monographs, book chapters, theses, conference proceedings, Components of a Research Publication: title, abstract, aims/objectives, hypothesis, rationale, methodology, results & discussion, key issues, acknowledgments, conflict of interest, bibliography, Research Metrics:

Journal metrics: Impact Factor (JCR), SNIP, SJR, IPP, CiteScore, Author metrics: h-index, g-index, i10-index

Unit 4: Data Analysis Using Chemistry Software and Statistical Tools (20 hrs)

Statistical Tools for Chemical Data Analysis: Descriptive statistics: mean, median, mode, standard deviation, variance, Correlation and regression analysis (linear, multiple), Analysis of Variance (ANOVA) for comparing datasets, Significance testing: t-test, χ^2 test, F-test, p-values, Error analysis: accuracy, precision, propagation of error, confidence limits, Case studies: statistical treatment of spectroscopic/analytical data, Software Applications in Chemistry: Origin: graph plotting, UV-Vis/Tauc plots, IR, XRD analysis, curve fitting, Mnova: NMR spectrum analysis, Gaussian & DFT basics: computational chemistry introduction, ORCA, GAMESS, GROMACS, Docking tools and applications in drug/ligand studies, SwissADME & related cheminformatics tools

Unit 5: Scientific Writing & Presentation (10 hrs)

Writing Research and Review Papers: structure, style, case examples,Project Proposals & Grant Writing: DST, SERB, CSIR schemes, Research Proposal Structure: title, abstract, hypothesis, objectives, methodology, expected outcomes, Budgeting & Resource Planning: cost estimation, equipment, manpower, feasibility, Research Timeline and Milestones: goal setting and deadlines, Oral & Poster Presentations: effective slide design, poster preparation, public speaking skills

References

1. C.R. Kothari & Gaurav Garg, *Research Methodology: Methods and Techniques*, New Age International.
2. J.W. Creswell & J.D. Creswell, *Research Design: Qualitative, Quantitative, and Mixed Methods Approaches*, SAGE.
3. D.C. Montgomery, *Design and Analysis of Experiments*, Wiley.
4. World Intellectual Property Organization (WIPO) – *Patent & IPR Guidelines* (official website).- https://www.wipo.int/portal/en/index.html
5. IP Government of India- https://ipindia.gov.in/
6. ACS (American Chemical Society) Publications – Author & Reviewer Resource Center.
7. RSC (Royal Society of Chemistry) Publishing – Guide for Authors.
8. Elsevier Author Hub – Researcher Academy (online).

9. Robert A. Day & Barbara Gastel, *How to Write and Publish a Scientific Paper*, Cambridge University Press
10. Silvia, Paul J., *How to Write a Lot: A Practical Guide to Productive Academic Writing*, APA.
11. DST, ANRF, CSIR – *Funding Guidelines and Proposal Formats* (official websites).
12. Origin / OriginPro – https://www.originlab.com/
13. Mnova (Mestrelab Research) – https://mestrelab.com/
14. SwissADME – Web tool access- http://www.swissadme.ch/index.php
15. GROMACS – https://www.gromacs.org/index.html
16. Gaussian – Official site (licensed)- https://gaussian.com/
17. ORCA Quantum Chemistry Package – https://orcaforum.kofo.mpg.de/index.php
18. GAMESS (US version) – https://www.msg.chem.iastate.edu/gamess/
19. Gabedit (GUI for QC codes) – https://gabedit.sourceforge.net/

Course 1

Physical Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Recall advanced concepts of thermodynamics, kinetics, quantum chemistry, and statistical mechanics governing chemical systems.

CO2: Explain molecular, electronic, and photochemical processes along with their theoretical and mechanistic foundations in reaction dynamics and energy transfer.

CO3: Apply computational, electrochemical, and spectroscopic tools to analyze chemical properties, energy materials, and nanostructured systems.

CO4: Analyze supramolecular interactions, molecular recognition, and solid-state structures using diffraction and characterization techniques.

CO5: Evaluate chemical processes in terms of thermodynamic efficiency, kinetics, and sustainability using principles of green and energy-efficient chemistry.

CO6: Design and synthesize advanced functional materials such as polymers, nanocomposites, and supramolecular systems for catalysis, energy, and environmental applications.

Content

Chapter 1: Advanced Thermodynamics and Statistical Mechanics (8 Hours)

- Advanced perspectives on the laws of thermodynamics; free energy and chemical potential.
- Partition functions and applications in evaluating thermodynamic properties.
- Ensembles in statistical mechanics: microcanonical, canonical, and grand canonical.
- Applications to phase equilibria, adsorption, and surface phenomena.
- Entropy, fluctuations, and cooperative transitions: statistical treatment.

Chapter 2: Chemical Kinetics and Photochemistry (8 Hours)

- Advanced rate laws and complex reaction mechanisms.
- Fast reactions, relaxation techniques, and transient kinetics.
- Photophysical and photochemical processes.
- Laser chemistry and photochemical energy conversion.
- Photochemical dynamics and applications in energy and environment.

Chapter 3: Molecular Quantum Chemistry and Computational Methods (10 Hours)

- Quantum principles: MO theory, perturbation theory, variational method.
- Ab initio and density functional theory (DFT).

- Basis sets, geometry optimization, electronic structure calculations.
- Computational tools for spectroscopy and thermodynamics.
- Open-source software (e.g., ORCA, GAMESS, Avogadro) for research applications.
- Applications in reactivity, catalysis, and molecular design.

Chapter 4: Electrochemistry, Nanoscience, and Energy Applications (8 Hours)

- Advanced electrochemistry: electrode kinetics and double-layer models.
- Electrochemical energy devices: fuel cells, batteries, supercapacitors.
- Nanochemistry: nucleation, growth, size effects, and synthesis techniques.
- Carbon nanomaterials, mesoporous materials, and nanostructured catalysts.
- Functional applications in energy storage and conversion.

Chapter 5: Supramolecular and Molecular Recognition Chemistry (8 Hours)

- Host–guest interactions and molecular recognition principles.
- Cyclodextrins, calixarenes, crown ethers.
- Supramolecular catalysis and transport processes.
- Chemosensors and electrochemical sensors.
- Chirality and stereoselective recognition.

Chapter 6: Solid State Chemistry and Crystallography (8 Hours)

- Crystal structures, symmetry, defects, and solid-state reactions.
- Band theory of solids, electronic and magnetic properties.
- X-ray diffraction and Rietveld refinement.
- Neutron and electron diffraction techniques (overview).
- Applications in materials science, nanoscience, and catalysis.

Chapter 7: Advanced Topics in Sustainable Chemistry (7 Hours)

- Twelve principles of green chemistry.
- Atom economy, energy efficiency, and benign solvents (water, ionic liquids).
- Microwave and ultrasonic methods in green synthesis.
- Carbon capture, utilization and storage (CCUS), biomass valorization.
- Thermodynamic and kinetic aspects of sustainable reactions.

Chapter 8: Polymer Chemistry – Structure, Kinetics, and Applications (3 Hours)

- Radical, step-growth, and living polymerizations.
- Molecular weight distribution, polydispersity index (PDI), Tg, and crystallinity.
- Characterization: GPC, DSC, TGA, viscometry.
- Advanced polymers: conducting, fire-retardant, biocompatible polymers; nanocomposites.

Suggested Reference Books:

1. P.W. Atkins and J. de Paula, *Atkins' Physical Chemistry*, Oxford Univ. Press.
2. Ira N. Levine, *Physical Chemistry*, McGraw Hill.
3. D.A. McQuarrie, *Statistical Mechanics*, Viva Books.
4. Ira N. Levine, *Quantum Chemistry*, Pearson.
5. Frank Jensen, *Introduction to Computational Chemistry*, Wiley.
6. A.J. Bard and L.R. Faulkner, *Electrochemical Methods*, Wiley.
7. P.W. Atkins & R.S. Friedman, *Molecular Quantum Mechanics*, Oxford.
8. J.W. Steed & J.L. Atwood, *Supramolecular Chemistry*, Wiley.
9. F.A. Cotton, *Chemical Applications of Group Theory*, Wiley.
10. P.T. Anastas & J.C. Warner, *Green Chemistry: Theory and Practice*, Oxford.
11. G. Odian, *Principles of Polymerization*, Wiley.
12. W.D. Callister, *Materials Science and Engineering*, Wiley.
13. T. Engel and P. Reid, *Physical Chemistry*, Pearson.
14. M. Ratner & D. Ratner, *Nanotechnology: A Gentle Introduction to the Next Big Idea*, Pearson.
15. IUPAC, *Quantities, Units and Symbols in Physical Chemistry (Green Book)*, IUPAC.

Course 2

Inorganic Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Recall fundamental concepts of bonding, structure, and defects in inorganic solids along with principles of bioinorganic, organometallic, and coordination chemistry.

CO2: Explain various synthesis, processing, and characterization techniques for inorganic materials and their relation to structure–property correlations.

CO3: Apply principles of thermodynamics, kinetics, and solid-state chemistry to analyze synthesis routes, phase formation, and microstructural evolution in inorganic and nanomaterials.

CO4: Analyze mechanisms of metal–ligand interactions, coordination reactions, and organometallic transformations using kinetic and electronic structure models.

CO5: Evaluate biochemical roles of essential metal ions and their coordination environments in catalysis, electron transfer, and enzymatic functions.

CO6: Design and interpret material characterization data to develop and report on advanced inorganic, porous, and nanocarbon materials with specific functional properties.

Content

Section-I: Chemistry of Inorganic Materials (02 Credit, 30 hours)

Chapter-1: Bonding in solids [03 hours]

Ionic Bonding - Ions and ionic radii, Ionic structures– general principles, The radius ratio rules, Borderline radius ratios and distorted structures, Lattice energy of ionic crystals, Kapustinskii's equation, The Born–Haber cycle and thermochemical calculations, (***Ref-1 125-142***); **Metallic Bonding and Band Theory:** Metallic Bonding and Band Theory, Band structure of metals, Band structure of insulators, Band structure of semiconductors: silicon, Band structure of inorganic solids (***Ref-1: 173-186***).

Chapter-2: Synthesis, Processing and Fabrication Methods [06 hours]

General Observations, **Solid State Reaction or Shake 'n Bake Methods**: Nucleation and growth, epitaxy and topotaxy, Practical considerations and some examples of solid state reactions, Combustion synthesis, Mechano synthesis; **Low Temperature or Chimie Douce Methods**: Alkoxide sol–gel method Generation of X-rays, Sol–gel method using oxyhydroxides and colloid chemistry, Citrate gel and Pechini processes, Use of homogeneous, single-source precursors, Hydrothermal and solvothermal synthesis, Microwave synthesis, Intercalation and deintercalation, Example of a difficult synthesis made possible by chimie douce methods: $BiFeO_3$, Molten salt synthesis, MSS; **Gas-Phase Methods**: Vapour-phase transport, Chemical vapour deposition-CVD, Sputtering and evaporation, Atomic layer deposition-ALD, Aerosol synthesis and spray pyrolysis; High-Pressure Methods; Crystal Growth ***(Ref-1: 187-228)***.

Chapter-3: Characterization Techniques of Material [06 hours]

Introduction to crystal structure: Lattice, Bravais Lattice, Unit Cell, Lattice Planes and Miller Indices, Indices of Directions, d-Spacing Formulae, Crystal Densities and Unit Cell Contents, (***Ref-1: 11-18***)

X-Ray Diffraction: Generation of X-rays, Interaction of X-rays with matter, Optical grating and diffraction of light, Crystals and diffraction of X-rays, X-ray diffraction methods, the powder method– principles and uses, Intensities, X-ray crystallography and structure determination– what is involved? (***Ref-1: 232-265, Refe-2 Relevant pages***): **Optical and Electron Microscopy Techniques:** Optical microscopy, Electron microscopy (only- Scanning electron microscopy and Transmission electron microscopy-TEM, and scanning transmission electron microscopy -STEM) (***Ref-1: 272-288, Refe-2 Relevant pages***); Spectroscopic Techniques **-** Vibrational spectroscopy: IR and Raman, Visible and ultraviolet (UV) spectroscopy, (***Ref-1: 291-298***), Thermal Analysis (***Ref-1: 314-320***).

Hands on activity: What is JCPDS data file and use of JCPDS data file for powder XRD analysis. Student will obtain powder XRD, SEM, SEM-EDS, TEM (2 examples each) from research paper and will perform detailed analysis. Will prepare report and submit to course coordinator.

Chapter-4: Defects and Non-stoichiometry [06 hours]

Point Defects: An Introduction, Defects and Their Concentration, Intrinsic Defects, Concentration of Defects, Extrinsic Defects, Ionic Conductivity in Solids, Solid Electrolytes, Fast-Ion Conductors: Silver Ion Conductors, Fast-Ion Conductors: Oxygen Ion Conductors, Fast-Ion Conductors: Sodium Ion Conductors, Applications of Solid Electrolytes, Batteries, Fuel Cells Oxygen Sensor, Oxygen Separation Membranes, Electrochromic Devices (***Ref-3: 201-238***)

Chapter-5: Microporous and Mesoporous Solids [06 hours]

Zeolites, Composition and Structure of Zeolites, Frameworks, Synthesis of Zeolites, Zeolite Nomenclature, Si/Al Ratios in Zeolites, Exchangeable Cations, Channels and Cavities, Structure Determination, Zeolites as Dehydrating Agents, Zeolites as Ion Exchangers, Zeolites as Adsorbents, Zeolites as Catalysts. (***Ref-3: 271-295***)

Chapter-6: Carbon Nanomaterials [03 hours]

Fullerenes, Carbon Nanotubes, Types of Carbon Nanotubes, Synthesis of Carbon Nanotubes, Growth Mechanism, Graphene, (Ref-4: 273-285).

References

1. Solid State Chemistry and its Applications, Second Edition, Student Edition, Anthony R. West, Wiley Publication.
2. Nanomaterials An Introduction to Synthesis, Properties and Applications, Dieter Vollath, Second Edition, Wiley-VCH.
3. Solid State Chemistry an introduction, Smart and Moore, Fourth Edition, 2012, Taylor & Francis Group,
4. Nanotechnology - principles and practices, Sulabha K. Kulkarni, 3rd Ed. Springer.

Section-II: Bioinorganic, Organometallic and Inorganic Reaction Mechanism (02 Credit, 30 hours)

Chapter-1: Bioinorganic Chemistry [15 hours]

Part-I: Sodium and Potassium Channels and Pumps: Introduction - Transport Across Membranes, Sodium Versus Potassium, Potassium Channels, Sodium Channels, the Sodium-Potassium Atpase, Active Transport Driven by Na^+ Gradients, Sodium/Proton Exchangers, Other Roles of Intracellular K^+. (Ref-1: 177-194, Ref-4).

Part-II: Magnesium Phosphate Metabolism and Photoreceptors: Introduction, Magnesium-Dependent Enzymes, Phosphoryl Group Transfer Kinases, Phosphoryl Group Transfer - Phosphatases, Stabilisation of Enolate Anions - The Enolase Superfamily, Enzymes of Nucleic Acid Metabolism, Magnesium and Photoreception. (Ref-1: 197-213, Ref-4).

Part-III: Calcium - Cellular Signalling: Introduction - Comparison of Ca^{2+} and Mg^{2+}, The Discovery of a Role for Ca^{2+} other than as a Structural Component, an Overview of Ca^{2+} Regulation and Signalling, Calcium Pumps, Intracellular Ca^{2+} Compartments, Ca^{2+} and Cell Signalling (Ref-1: 215-228, Ref-4).

Part-IV: Zinc-Lewis Acid and Gene Regulator: Introduction, Mononuclear Zinc Enzymes: Carbonic Anhydrase, Alcohol Dehydrogenases; other Mononuclear Zinc Enzymes, Metalloproteinases Multinuclear and Co-catalytic Zinc Enzymes, Zinc Fingers DNA- and RNA-Binding Motifs (Ref-1: 229-246, Ref-4).

Part-V: Iron: Essential for Almost All Life: Introduction, Iron Chemistry, Iron and Oxygen, The Biological Importance of Iron, Biological Functions of Iron-Containing Proteins, Haemoproteins: Oxygen Transport, Activators of Molecular Oxygen, Iron-Sulfur Proteins. (Ref-1: 247-266, Ref-4)

Part-VI: Copper - Coping with Dioxygen: Introduction Copper Chemistry and Biochemistry: Type 1 Blue Copper Proteins - Electron Transport; Copper-Containing Enzymes in Oxygen Activation and Reduction: Type 2 Copper Proteins; Mars and Venus - The Role of Copper in Iron Metabolism (Ref-1: 279-295, Ref-4)

Part-VII: Manganese e Oxygen Generation and Detoxification: Introduction: Mn Chemistry and Biochemistry, Photosynthetic Oxidation of Water - Oxygen Evolution, Mn^{2+} and Detoxification of Oxygen Free Radicals, Nonredox di-Mn Enzymes - Arginase. (Ref-1: 311-320, Ref-4).

Chapter-2: Reactions of Coordination Compounds [07 hours]

Kinetics Overview, Octahedral Substitution Reactions, Associative(A)Mechanism Interchange(I)Mechanism, Dissociative(D)Mechanism, Square Planar Substitution Reactions, Electron Transfer Reactions, Inorganic Photochemistry, Photochemistry of Chromium(III)Ammine Compounds, Light-Induced Excited State Spin Trapping in Iron(II)Compounds, MLCT Photochemistry in Pentaammineruthenium(II)Compounds, Photochemistry and Photophysics of Ruthenium(II) Polypyridyl Compounds, (Ref-2: 573- 622, Ref-3 Relevant Pages)

Chapter-3: Structure and Bonding and reactions in Organometallic Compounds [08 hours]

Part-A: Introduction to Organometallic Chemistry, ElectronCountingandthe18-Electron Rule, Carbonyl Ligands, Nitrosyl Ligands, Hydride and Dihydrogen Ligands, Phosphine Ligands, Ethylene and Related Ligands, Cyclopentadiene and Related Ligands, Carbenes, Carbynes, and Carbidos. (Ref-2: 627-651, Ref-3 Relevant Pages)

Part-B: Reactions of Organometallic Compounds: Some General Principles, Organometallic Reactions Involving Changes at the Metal, Ligand Substitution Reactions, Oxidative Addition and Reductive Elimination, Organometallic Reactions Involving Changes at the Ligand, Insertion and Elimination Reactions, Nucleophilic Attack on the Ligands, Electrophilic Attack on the Ligands, Metathesis Reactions, π-Bond Metathesis, Ziegler–Natta Polymerization of Alkenes, σ-Bond Metathesis, Commercial Catalytic Processes, Catalytic Hydrogenation, Hydroformylation, Wacker–Smidt Process, Monsanto Acetic Acid Process, Organometallic Photochemistry, Photosubstitution of CO, Photoinduced Cleavage of Metal–Metal Bonds, Photochemistry of Metallocenes, The Isolobal Analogy and Metal–Metal Bonding in Organometallic Clusters, (Ref-2: 655 – 689, Ref-3 Relevant Pages)

References

1. **Biological Inorganic Chemistry a New Introduction to Molecular Structure and Function,** Robert R. Crichton, 2nd Ed (2012), Elsevier.
2. **Principles of Inorganic Chemistry**, Brian W. Pfennig, Wiley, 2015.
3. **Inorganic Chemistry**, Duward Shriver, Mark Weller, Tina Overton, Jonathan Rourke, Fraser Armstrong, W. H. Freeman and Company, 6th Ed.
4. **Comprehensive Coordination Chemistry II**. Bio-coordination Chemistry. Vol.8, L. Que, Jr., W.B. Tolman, Elsevier Science (2003).

Course 3

Organic Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Recall important named reactions, synthetic methodologies, and functional group transformations involved in modern organic synthesis.

CO2: Explain mechanisms of coupling, multicomponent, and pericyclic reactions, as well as the role of green solvents and catalysts in sustainable synthesis.

CO3: Apply synthetic strategies for the construction of heterocyclic and bioactive molecules using classical and modern organic methodologies.

CO4: Analyze emerging techniques—organometallic, photoredox, flow, nanocatalysis, and computational tools—to design efficient synthetic pathways.

CO5: Evaluate structural and electronic properties of organic and inorganic systems using advanced spectroscopic techniques such as UV–Vis, IR, NMR, and Mass spectrometry.

CO6: Integrate multi-spectroscopic data (UV–Vis, IR, NMR, MS) to elucidate molecular structures and propose complete reaction mechanisms for newly synthesized compounds.

Content

Section I: Organic Chemistry Reactions (30 hours)

Chapter 1: Named Reactions & Synthetic Methodologies (8 hours)

Importance of Named reactions in drug discovery, Case studies: Chalcone synthesis and Click chemistry; C–C and C–N Coupling Reactions: Mechanistic aspects, Heck Reaction, Suzuki–Miyaura Coupling, Sonogashira Coupling, Buchwald–Hartwig Amination, Negishi & Stille Couplings, Case studies of each reaction; Multicomponent reactions (MCRs): Biginelli, Ugi, Passerini; Pericyclic reactions: Overview, Diels–Alder reaction; Role of green solvents (ionic liquids, DES, water, solvent-free conditions)

Chapter 2: Functional Group Transformations (7 hours)

Classical & Modern Oxidations: Review of common oxidation processes ($KMnO_4$, Cr(VI) reagents) – limitations (toxicity and selectivity); Swern Oxidation, Dess–Martin Periodinane, TEMPO-mediated Oxidation, Oxone, Photocatalytic Oxidations; Classical & Modern Reductions: $NaBH_4$, $LiAlH_4$, $LiBH_4$, DIBAL-H, Red-Al, Borane, Super-Hydrides ($LiEt_3BH$, L-Selectride, K-Selectride), Dissolving metal reductions; Protecting group strategies & orthogonal protection–deprotection in multistep synthesis; Organocatalysis and asymmetric synthesis: Asymmetric aldol reaction.

Chapter 3: Heterocyclic and Bioactive Molecule Synthesis (8 hours)

Synthetic approaches for heterocycle synthesis: Hantzsch Dihydropyridine Synthesis, Paal–Knorr Synthesis Furan, Pyrrole and thiophene, Hantzsch Thiazole Synthesis, thiazole, Fischer Indole Synthesis, Skraup Synthesis; Reactivity: Electrophilic and nucleophilic.

Application of each given heterocyle in drug discovery and materials chemistry

Chapter 4: Emerging Tools & Techniques in Organic Synthesis (7 hours)

Organometallic reagents and their role in synthesis (Grignard, organolithium, organozinc, organoboron), Photoredox catalysis and visible-light-mediated transformations, Flow chemistry and high-throughput experimentation in research labs, Applications of nanocatalysts in organic synthesis, Introduction to computational organic chemistry (reaction mechanism studies using DFT)

Section II: Advanced Spectroscopic Methods (30 hours)

Chapter 5: UV–Visible Spectroscopy in Research (5 hours)

Electronic transitions and chromophore-auxochrome effects, Solvent effects, hyper- and hypochromic shifts, Applications in drug/nanomaterial characterization, UV-Vis in kinetics, stability studies, and band gap determination (nanomaterials, photocatalysts), Case studies: charge transfer spectra (Case Study Examples: $Fe(bipy)_3]^{2+}$, $[Ru(bipy)_3]^{2+}$, intense MLCT bands in dye-sensitized solar cells, Hemoproteins (cytochrome c, hemoglobin); Effect of conjugation on λmax: Case Study Examples: β-carotene, Azo dyes, Anthocyanins, Graphene oxide / carbon dots

Chapter 6: Infrared Spectroscopy in Research (5 hours)

Dispersive vs Fourier Transform Infrared (FT-IR), ATR, Diffuse Reflectance & Solid-State IR, Sample preparation: KBr pellets, NaCl plates, Nujol mull, thin film, ATR probes, Hyphenated techniques: TGA–IR, GC–IR, LC–IR; Vibrational modes, factors affecting frequencies, correlations, Identification of functional groups in complex molecules and Interpretation of IR spectra, Applications: monitoring organic synthesis, hydrogen bonding, supramolecular interactions, etc

Chapter 7: Nuclear Magnetic Resonance Spectroscopy (15 hours)

^{1}H NMR: Basic principle, chemical shift, spin-spin coupling, multiplicity, integration, dynamic NMR, first order and second NMR, D_2O exchange; ^{13}C NMR: basic principle and comparison with ^{1}H NMR, proton coupled and decoupled spectra, chemical shifts; Solvents used in NMR; coupling of ^{1}H and ^{13}C with ^{19}F and ^{31}P; Advanced NMR: 2D techniques (DEPT, COSY, HETCOR, HSQC, HMBC, NOESY) for structure elucidation; Applications in stereochemistry determination, conformational analysis, Tautomerism studies, Solid-state NMR, Case studies from drug discovery

Chapter 8: Mass Spectrometry in Research (5 hours)

Basic principle, Ionization techniques: EI, Chemical ionization, ESI, MALDI; Mass analyzers: TOF, Q-TOF, Orbitrap, Base peak and molecular ion peak, Nitrogen rule, rule of 13, Mclafferty, High-resolution MS in molecular formula determination, isotopic peaks in mass spectrometry (Cl and Br only).

References

1. Kürti & Czakó – *Strategic Applications of Named Reactions in Organic Synthesis*, 1st Ed., 2005
2. Jie Jack Li – *Name Reactions*, 5th Ed., 2021
3. Carey & Sundberg – *Advanced Organic Chemistry (Parts A & B)*, 5th Ed., 2007
4. Smith & March – *March's Advanced Organic Chemistry*, 7th Ed., 2013
5. Warren & Wyatt – *Organic Synthesis: The Disconnection Approach*, 2nd Ed., 2008
6. Greene & Wuts – *Protective Groups in Organic Synthesis*, 5th Ed., 2014
7. Bansal – *Heterocyclic Chemistry*, 6th Ed., 2017
8. Joule & Mills – *Heterocyclic Chemistry*, 5th Ed., 2010
9. MacMillan & Yoon – *Photoredox Catalysis in Organic Chemistry*, ACS, 2016
10. Seeberger & Gilmore – *Flow Chemistry*, RSC Publishing, 2017
11. Pavia, Lampman, Kriz & Vyvyan – *Introduction to Spectroscopy*, 5th Ed., 2014
12. Kemp – *Organic Spectroscopy*, 3rd Ed., 1991
13. Claridge – *High-Resolution NMR Techniques in Organic Chemistry*, 3rd Ed., 2016
14. Keeler – *Understanding NMR Spectroscopy*, 2nd Ed., 2010

Course 4

Material Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Recall the history, scope, and fundamental concepts of nanoscience, crystal structures, and types of bonding in solids.

CO2: Explain the classification, formation, and unique properties of nanostructured materials in relation to their crystal geometry and bonding nature.

CO3: Apply physical, chemical, and biological methods for the synthesis of nanomaterials and correlate process parameters with resulting material properties.

CO4: Analyze the electronic structure and behavior of semiconductors, including doping effects, charge carrier dynamics, and device characteristics.

CO5: Evaluate the structure–property relationships of nanomaterials using various advanced characterization techniques such as XRD, SEM, TEM, FTIR, UV–Vis, Raman, and XPS.

CO6: Integrate synthesis, characterization, and application knowledge to design nanomaterials for specific applications in energy, environment, electronics, catalysis, and healthcare.

Content

Section-I (30 hours)

Chapter 1: The Big World of Nanomaterials **[4 Hours]**

History and Scope, Can Small Things Make a Big Difference? Classification of Nanostructured Materials, Fascinating Nanostructures, Nature: The Best Nanotechnologist, Challenges and Future Prospects.

Chapter 2: Crystal structures **[14 Hours]**

Introduction, Unit Cells and Crystal Systems, Symmetry, Symmetry and Choice of Unit Cell, Lattice, Bravais Lattice, Lattice Planes and Miller Indices, Indices of Directions, d-Spacing Formulae, Crystal Densities and Unit Cell Contents, Description of Crystal Structures, Close Packed Structures – Cubic and Hexagonal Close Packing, Relationship between Cubic Close Packed and Face Centred Cubic, Hexagonal Unit Cell and Close Packing, Density of Close Packed Structures, Unit Cell Projections and Atomic Coordinates, Unit Cell Projections and Atomic Coordinates, Structures Built of Space-Filling Polyhedra, Some Important Structure Types: Rock salt (NaCl), zinc blende or sphalerite (ZnS), fluorite (CaF_2), antifluorite (Na_2O), Diamond, Wurtzite (ZnS) and nickel arsenide (NiAs), Caesium chloride (CsCl), Other AX structures, Anatase, Brookite and Rutile (TiO_2), cadmium iodide (CdI_2), cadmium chloride

($CdCl_2$) and caesium oxide (Cs_2O), Perovskite ($SrTiO_3$), Rhenium trioxide (ReO_3), perovskite tungsten bronzes, tetragonal tungsten bronzes, Spinel, Olivine, Corundum, ilmenite and $LiNbO_3$, Fluorite-related structures and pyrochlore, Silicate structures

Chapter 3: Bonding in Solids **[6 Hours]**

Overview: Ionic, Covalent, Metallic, van der Waals and Hydrogen Bonding in Solids, Ionic Bonding, Covalent Bonding, Metallic Bonding and Band Theory, Band structure of metals, insulators, semiconductors, inorganic solids.

Chapter 4: Types of Nanomaterials and Their Properties **[6 Hours]**

Introduction, Clusters, Semiconductor Nanoparticles, Plasmonic Materials, Nanomagnetism, Microstructure and defects in nanocrystalline materials (Dislocations, Twins, stacking faults and voids, Grain boundaries, triple junctions and disclinations), Effect of nano-dimensions on materials behaviour (Elastic properties, Melting point, Diffusivity, Grain growth characteristics, Enhanced solid solubility, Magnetic properties, Electrical properties, Optical properties, Thermal properties, Mechanical properties)

Section-II (30 hours)

Chapter 1: Synthesis of Nanomaterials **[4 Hours]**

Physical Methods: Mechanical Methods High Energy Ball Milling, Melt Mixing, Chemical Vapour Deposition (CVD), Electric Arc Deposition **Chemical Methods:** Sol-Gel Method, Hydro/Solvothermal Synthesis, Sonochemical Synthesis, Microwave Synthesis, Combustion Synthesis and co-precipitation. **Biological Methods:** Synthesis Using Microorganisms, Synthesis Using Plant Extracts, Use of Proteins, Templates Like DNA, S-Layers etc., Synthesis of Nanoparticles Using DNA.

Chapter 2: Semiconductors **[8 Hours]**

Introduction, Intrinsic Semiconductors, Effective mass, Recombination of electrons and holes, Extrinsic Semiconductors, N-type semiconductor, P-type semiconductor, effect of temperature, effect of doping, donor and acceptor states, Fermi level in extrinsic semiconductor, Semiconductor Devices, P-N junction, forward and reverse biasing, Volt-Ampere characteristics of P-N Junction, effect of temperature on PN Diodes, Zener diodes, Tunnel diode, Photodiode, Solar cells, photovoltaic effect and solar cells, Light emitting diodes, Liquid crystal display(LCD)

Chapter 3: Material Characterization Techniques **[12 Hours]**

Chemical and Structural Analyses

History, Mechanism, Advantages and Disadvantages, Applications of Raman Spectroscopy, Fourier Transform Infrared Spectroscopy, Ultraviolet–Visible Spectroscopy, X-Ray Photoelectron Spectroscopy, Diffuse Reflectance Infrared Fourier Transform Spectroscopy, X-Ray Diffraction, Nuclear Magnetic Resonance, Scanning Electron Microscopy, Transmission Electron Microscopy

Coupled Characterization Techniques

Advantages and Disadvantages, Applications of Scanning Electron Microscopy Coupled with Energy-Dispersive X-Ray for Material Characterization, Ultraviolet–Visible Coupled with Cyclic Voltammetry for Material Characterization**.**

Chapter 4: Applications of Nanomaterials [6 Hours]

Nano-Electronics, Quantum dot lasers, Photonic crystals, Micro- and Nano-Electromechanical Systems (MEMS/NEMS), Nanosensors, Nanocatalysts, Food and Agriculture Industry, Cosmetics and Consumer Goods, Structure and Engineering, Automotive Industry, Water Treatment and the Environment, Nano-Medical Applications, Textiles, Paints, Energy, Defence and Space Applications, Structural Applications.

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1. Textbook of Nanoscience and Nanotechnology, by B.S. Murty, P. Shankar, Baldev Raj, B B Rath, James Murday, Heidelberg, 1st Edition (2013), Springer Publications. https://doi.org/10.1007/978-3-642-28030-6
2. Nanotechnology: Principles and Practices by Sulabha K. Kulkarni, 3rd Edition (2014), Springer publications. https://doi.org/10.1007/978-3-319-09171-6
3. Solid State Chemistry and its Applications by Anthony R. West, Second Edition, Student Edition, ISBN: 978-1-119-94294-8 (Link)
4. Material Characterization Techniques and Applications by Euth Ortiz Ortega, Hamed Hosseinian, Ingrid Berenice Aguilar Meza, María José Rosales López, Andrea Rodríguez Vera, Samira Hosseini, in series Progress in Optical Science and Photonics, 1st Edition, (2022), Springer publication. https://doi.org/10.1007/978-981-16-9569-8
5. Material Science by S.L.Kakani and Amit Kakani, New Age International Limited, ISBN (13) : 978-81-224-2656-4 (Link)
6. Material Characterization Techniques and Applications by Euth Ortiz Ortega, Hamed Hosseinian, Ingrid Berenice Aguilar Meza, María José Rosales López, Andrea Rodríguez Vera, Samira Hosseini, in series Progress in Optical Science and Photonics, 1st Edition, (2022), Springer publication. https://doi.org/10.1007/978-981-16-9569-8
7. Characterization Techniques for Nanomaterials by Imalka Munaweera, M.L. Chamalki Madhusha, 1st Edition 2023, CRC Press. https://doi.org/10.1201/9781003354185

Course 5

Advanced Techniques in Analytical Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Demonstrate advanced understanding of the physicochemical principles, selection rules, and electronic/magnetic interactions governing modern spectroscopic and chromatographic techniques.

CO2: Explain the operating principles, instrumentation architecture, detection systems, calibration strategies, performance parameters, and analytical limitations of major analytical instruments.

CO3: Apply advanced separation, spectroscopic, mass spectrometric, and thermal analytical methods to solve complex multidisciplinary research problems in chemistry, materials science, biochemistry, environment, and pharmaceuticals.

CO4: Analyze and interpret complex multidimensional datasets using chemometrics, multivariate statistics, spectral deconvolution, and modern computational data-handling tools.

CO5: Critically evaluate the scientific literature, recent advancements, challenges, and future trends in analytical chemistry, identifying research gaps and proposing solutions.

CO6: Integrate multiple analytical platforms (e.g., HPLC-MS, GC-MS, NMR-MS, TGA-FTIR, DSC-TGA) to establish structure, composition, purity, kinetics, and mechanistic understanding of advanced chemical systems.

Content

Section I

Chapter 1: Fundamentals of Spectroscopy **(8 Hours)**

Quantum basis of radiation–matter interaction, Selection rules & transition probabilities, Line broadening (Doppler, collision, relaxation), Signal-to-noise optimization, High-resolution & time-resolved spectroscopy, Detector technologies, Statistical data treatment

Chapter 2: UV–Visible, IR & Raman Spectroscopy **(8 Hours)**

Advanced Beer–Lambert Law, deviations, Diode-array & multiwavelength detection, Chemometric spectral deconvolution, Vibrational theory & normal mode analysis, Instrumentation: UV–Vis, ATR-FTIR, FT-Raman, SERS, Spectral pre-processing & multivariate interpretation, Applications in nanomaterials, biological, forensic & environmental systems

Chapter 3: Nuclear Magnetic Resonance Spectroscopy (7 Hours)

Nuclear spin theory & relaxation mechanisms, 2D and multidimensional NMR (COSY, HSQC, NOESY, EXSY, DOSY), Solid-state MAS NMR, In situ NMR, Metabolomics & molecular dynamics, Automated spectral interpretation & data analytics

Chapter 4: Mass Spectrometry, AAS and Thermal Analysis (7 Hours)

ICP-OES, ICP-MS, AAS, Excitation/ionization physics & interference corrections, Isotope ratio MS & high-resolution analyzers (Orbitrap, FT-ICR, Q-TOF), Tandem MS & fragmentation rules, Construction of spectral libraries & peak clustering, TGA, DSC, DTA fundamentals, Thermal characterization of polymers, pharmaceuticals, catalysts & materials

Section II

Chapter 5: Principles of Separation Science (8 Hours)

Van Deemter theory & efficiency, Resolution optimization & peak capacity modelling, Orthogonal & multidimensional separations, Hyphenation interfaces & design, Fundamental aspects applicable to GC, HPLC, IC, CE & TLC

Chapter 6: Gas Chromatography & Hyphenated GC Systems (8 Hours)

Capillary/open tubular columns, Ionic-liquid stationary phases, 2D GC×GC, Injection methods: split, splitless, on-column, Detectors: FID, TCD, ECD, MS, IRMS, Chromatographic deconvolution, Applications: environment, petrochemicals, pharmaceuticals, and food

Chapter 7: Liquid Chromatography – HPLC & UHPLC (7 Hours)

Columns: monolithic, superficially porous, core–shell, Gradient modeling & retention prediction, DoE-based method development, Detectors: UV, fluorescence, RI, MS, Impurity profiling, stress studies & stability testing, Applications in pharmaceuticals & bioproducts

Chapter 8: Ion Chromatography, Electrophoresis & Planar Chromatography (7 Hours)

Ion-exchange principles, Suppressed & nonsuppressed conductivity detection, Capillary electrophoresis & CE–MS coupling, HPTLC automation & 2D planar chromatography, Chemometric image processing, TLC–MS interfaces, Trace analyses in biotechnology, metabolomics & inorganic chemistry

References

1. Banwell, C.N. & McCash, E.M. (2006). Fundamentals of Molecular Spectroscopy, 4th Edition, Tata McGraw-Hill, New Delhi.
2. Skoog, D.A., Holler, F.J. & Crouch, S.R. (2007). Principles of Instrumental Analysis, 7th Edition, Cengage Learning India.

3. Willard, Merritt, Dean & Settle (1991). Instrumental Methods of Analysis, 7th Edition, CBS/IBH Book House, New Delhi.
4. Kakkar, R. (2015). Atomic and Molecular Spectroscopy: Concepts and Applications, Cambridge University Press.
5. de Hoffmann, E. & Stroobant, V. Mass Spectrometry: Principles and Applications, 3rd Edition, Wiley-VCH.
6. Holčapek, M. & Byrdwell, W. (Editors). Handbook of Advanced Chromatography / Mass Spectrometry Techniques, Latest Edition, Wiley/CRC Press.
7. Günzler, H. & Williams, A. (Editors). Handbook of Analytical Techniques (Two-Volume Set), Latest Edition, Wiley-VCH/Dattani Book Agency.
8. IUPAC. Compendium of Analytical Nomenclature (Orange Book), Latest Edition, IUPAC Publishing.

Course 6

Green Chemistry

Credits: 04 (60 Hours)

Course Outcomes

CO1: Explain the fundamental concepts, need, and goals of Green Chemistry in relation to sustainable development and environmental protection.

CO2: Analyze and apply the twelve principles of Green Chemistry to design safer, atom-economical, and waste-minimized chemical syntheses.

CO3: Evaluate the role, advantages, and limitations of green solvents (water, supercritical CO_2, ionic liquids, PEG, fluorous media) and eco-benign reagents in organic transformations.

CO4: Demonstrate understanding of green catalytic systems—such as phase-transfer catalysts, polymer-supported reagents, and crown ethers—and their applications in sustainable synthesis.

CO5: Apply alternative energy-assisted methods (microwave, ultrasound, and photochemical techniques) to develop efficient and environment-friendly chemical processes.

CO6: Critically assess industrial and research-based case studies (e.g., Ibuprofen, adipic acid, nanoparticles) to design innovative, safe, and sustainable synthetic strategies aligned with the principles of Green Chemistry.

Content

Chapter 1: Introduction to Green Chemistry **(06 Hours)**

[Ref 1-5]

- What is Green Chemistry?
- Need for Green Chemistry
- Goals of Green Chemistry
- Definitions and Concepts:
  - Green Chemistry
  - Sustainable consumption of resources

Chapter 2: Principles of Green Chemistry and Planning a Chemical Synthesis

(12 Hours)

[Ref 1-5]

- The Twelve Principles of Green Chemistry (overview & definition)
- Designing and Planning a Green Synthesis
- Use of Environmentally Benign Solvents
- Avoidance of Unnecessary Derivatization

- Use of Catalysts
- Polymer-Supported Reagents
- Waste/By-product Prevention
- Atom Economy and Maximum Incorporation of Raw Materials
- **Case Studies of Green Synthesis**:
    - Adipic Acid
    - Sebacic Acid
    - Ibuprofen
    - Quinoxalines

Chapter 3: Organic Synthesis in Benign Green Solvents (12 Hours) [Ref 1-4, 6, 7]

- Sustainable Development and Cleaner Production
- Green Synthesis of Nanoparticles
- **Organic Synthesis in Water**:
    - Pericyclic Reactions
    - Wittig–Horner Reaction
    - Michael Reaction
    - Mannich-Type Reactions
    - Knoevenagel Reaction
    - Strecker Synthesis
    - Oxidations, Reductions, C–C Bond Formations in Aqueous Media
- **Organic Synthesis in Supercritical CO_2**:
    - Asymmetric Catalysis
    - Diels–Alder Reaction
    - Photochemical Reactions
    - Acid-Catalyzed Reactions
    - Coupling Reactions

Chapter 4: Organic Synthesis using Ionic Liquids and Fluorous Solvents (10 Hours) [Ref 1-4, 8-9]

- Introduction, Types, and Preparation of Ionic Liquids
- Applications of Ionic Liquids in Reactions:
    - Baylis–Hillman Reaction
    - Knoevenagel Condensation
    - Claisen–Schmidt Condensation

- Horner–Wadsworth–Emmons Reaction
- C–C and C–O Bond Formations
- Biginelli Reaction

- **Fluorous Solvents**:
  - Introduction and Characteristics of Perfluorous Liquids
  - Perfluorinated Catalysts

Chapter 5: Organic Synthesis using PEG, Green Catalysts, and Crown Ether (10 Hours)

[Ref 1-4, 10, 11]

Introduction and Characteristics of Polyethylene Glycol (PEG)

- PEG in Organic Reactions
- PEG as Phase-Transfer Catalyst (PTC):
  - Asymmetric Dihydroxylation of Olefins
  - Regioselective Heck Reaction
  - Baylis–Hillman Reaction
  - Suzuki Cross-Coupling Reaction
  - Synthesis of Azo Compounds
- Phase Transfer Catalysts (PTC):
  - Types and Advantages
  - Applications in Organic Synthesis
- Synthetic Applications of Crown Ether

Chapter 6: Alternate Energy Processes in Chemical Synthesis (10 Hours)

[Ref 1-4, 12-14]

1. **Microwave-Assisted Organic Synthesis**
   - Reactions in Water
   - Reactions in Organic Solvents
   - Reactions in Solid State
2. **Ultrasound-Assisted Organic Synthesis**
   - Types of Sonochemical Reactions
   - Homogeneous Sonochemical Reactions
   - Heterogeneous Liquid–Liquid Reactions
   - Heterogeneous Solid–Liquid Reactions
3. **Photo-Induced Organic Synthesis**
   - Introduction and Photochemical Reactions

- Principal Industrial Applications of Photochemistry

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1. (a) A. S. Matlack: Introduction to Green Chemistry, Marcel Deckkar (2001). (b) Anastas, P. T., Warner, J. Green Chemistry: Theory and Practice; Oxford University Press: London, (1998). (c) Lancaster, M. *Green Chemistry: An Introductory Text*. RSC Publishing.
2. Mukesh Doble, Anil Kumar Kruthiventi, in Green Chemistry and Engineering, (2007).
3. V. K. Ahluwalia & M. R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005);
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6. Poliakoff, M., Fitzpatrick, J. M., Farren, T. R., & Anastas, P. T. "Green Chemistry: Science and Politics of Change," *Science*, 2002.
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9. Horváth, I. T., *Fluorous Chemistry*. Springer
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12. Loupy, A. *Microwaves in Organic Synthesis*. Wiley-VCH.
13. Mason, T. J. *Sonochemistry*. Oxford University Press.
14. Turro, N. J. *Modern Molecular Photochemistry*.

Course 7

Drug Design and Development

Credits: 04 (60 Hours)

Course Outcomes

CO1: Explain the fundamental concepts of drug discovery and development

CO2: Apply knowledge of pharmacology, medicinal chemistry, and molecular biology for identifying potential drug targets and designing lead compounds.

CO3: Analyse lead optimization strategies, ADME properties, and case studies of successful drugs in order to evaluate structure–activity relationships.

CO4: Assess the strengths and limitations of computational approaches such as QSAR, docking, pharmacophore modelling, and AI-driven drug design.

CO5: Design innovative research strategies integrating natural product chemistry, synthetic approaches, and computational tools for novel drug discovery.

CO6: Formulate independent and translational research ideas addressing unmet therapeutic needs, while considering ethical, regulatory, and sustainability perspectives.

Content

Chapter 1: Introduction to Drug Discovery & Development (06 hours)

1. Overview of Human Diseases and Therapeutic Needs
2. Historical Perspectives and Medicines that Changed the World
3. Introduction to Drug Development Pipeline (Discovery → Preclinical → Clinical → Market)

Chapter2: Drug Targets and Mechanisms (08 hours)

1. Receptors, Enzymes, Ion Channels, and Nucleic Acids as Targets
2. Signal Transduction Pathways and Mechanisms of Drug Action
3. Target Validation Approaches
4. Case Studies: Antibiotics, Anticancer, Antiviral Targets

Chapter 3: Lead Discovery and Optimization (10 hours)

1. Sources of Leads: Natural Products, Synthetic Compounds, Biologics
2. High Throughput Screening (HTS) and Combinatorial Chemistry
3. Structure–Activity Relationship (SAR) Studies
4. Prodrugs and Drug Metabolism in Lead Optimization
5. Case Study: Aspirin, Penicillin, Statins

Chapter 4: Computational Approaches in Drug Design (12 hours)

1. Role of Bioinformatics and Chemo informatics in Drug Discovery
2. Molecular Modelling: Docking and Scoring Functions
3. Quantitative Structure–Activity Relationship (QSAR) Methods
4. Pharmacophore Modelling and Virtual Screening
5. Computer-Aided Drug Design (CADD) Success Stories
6. AI, Machine Learning, and Big Data in Modern Drug Discovery

Chapter 5: ADME and Toxicology (06 hours)

1. Pharmacokinetics: Absorption, Distribution, Metabolism, Excretion (ADME)
2. Drug Toxicity: Types, Mechanisms, and Prediction Models
3. In vitro and In vivo Screening for ADME-T Properties

Chapter 6: Preclinical and Clinical Development (10 hours)

1. Preclinical Testing: Animal Models, Ethics, GLP Guidelines
2. Clinical Trials: Phases I–IV, Design and Conduct
3. Regulatory Affairs: FDA, EMA, CDSCO, and ICH Guidelines
4. Intellectual Property Rights, Patents, and Generic Drugs
5. Drug Repurposing and Orphan Drugs

Chapter 7: Advanced Trends and Future Perspectives (08 hours)

1. Biopharmaceuticals and Monoclonal Antibodies
2. Gene Therapy, RNA-based Drugs, and Nanomedicine
3. Personalized and Precision Medicine
4. Future Directions: Green Chemistry, Sustainability, and AI-driven Drug Design

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2. Silverman, R. B. & Holladay, M. W. *The Organic Chemistry of Drug Design and Drug Action*.
3. Hill, R. G. *Drug Discovery and Development: Technology in Transition*.
4. Barret, A. & Rawlings, N. D. *Proteases and Their Inhibitors in Drug Discovery*.
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