



## Department of Chemistry

### Ph.D. Course Work

(Applicable for the scholars admitted from the AY: 2024-25)

The credit requirement for the Ph.D. course work is a minimum of 12 credits including the courses on 'Research Methodology' and 'Research and Publication Ethics' for 2 credits each. The candidate must complete two domain-specific courses of 3 credits each, recommended by the respective Department Research Committee (DRC). These courses can be completed through MOOCs.

The candidate must present two research seminars before the completion of course work, typically within the first year. The first research seminar shall be before the end of first semester on introduction to the proposed research work, and the second seminar shall be before the end of the second semester or after the completion of course work on the research proposal, as per the format provided. Each research seminar will have one credit weightage. The course structure is presented in Table 1 and list of domain-specific courses is presented in Table 2.

**Table 1: Course Structure**

S.No.	Course Code	Name of the Course	Credit (s)
1	246UC001	Research Seminar -I	1
2	246UC002	Research Seminar -II	1
3	246UC003	Research Methodology	2
4	246UC004	Research and Publication Ethics	2
5	-	Domain Specific Course -I	3
6	-	Domain Specific Course -II	3
<b>Total</b>			<b>12</b>

### List of Domain-Specific Courses

S. No.	Course Code	Name of the Course
1	246CH001	Theoretical and Computational Chemistry-Methods and Applications.
2	246CH002	Interpretative Molecular Spectroscopy
3	246CH003	Advanced Organic Synthesis: Oxidation, Reduction, and C-C Bond Formation Strategies for Natural Product Synthesis
4	246CH004	Chemistry of Nanomaterials
5	246CH005	Nuclear Chemistry in Research and Industry-Techniques and Innovations.
6	246CH006	Sensor Technologies in Chemistry-Principles and Applications.
7	246CH007	Organic Transformations and Reagents-Catalysis, Selectivity, and Functional Group Interconversions.
8	246CH008	Medicinal Chemistry
9	246CH009	Advanced Green Chemistry-Sustainable Strategies and Innovations in Chemical Processes.
10	246CH010	Environmental Quality Monitoring & Analysis
11	246CH011	Industrial Wastewater Treatment
12	246CH012	Spectroscopy for Structural Elucidation
13	246CH013	Reagents in Organic Synthesis
14	246CH014	Separation Techniques and Bioanalytical Chemistry

## Research Methodology

Course Code: 246UC003

### UNIT -I:

#### Research Design

Overview of research process and design, Use of Secondary and exploratory data to answer the research question, Qualitative research, Observation studies, Experiments and Surveys. Case Studies.

### UNIT-II:

#### Data Collection and Sources

Measurements, Measurement Scales, Questionnaires and Instruments, Sampling and methods. Data - Preparing, Exploring, examining and displaying.

### UNIT-III:

#### Data Analysis and Reporting

Overview of Multivariate analysis, Hypotheses testing and Measures of Association. Presenting Insights and findings using written reports and oral presentation.

### UNIT-IV:

#### Intellectual Property Rights

Intellectual Property – The concept of IPR, Evolution and development of concept of IPR, IPR development process, Trade secrets, utility Models, IPR & Bio diversity, Role of WIPO and WTO in IPR establishments, Right of Property, Common rules of IPR practices, Types and Features of IPR Agreement, Trademark, Functions of UNESCO in IPR maintenance.

### UNIT-V:

#### Patents

Patents – objectives and benefits of patent, Concept, features of patent, Inventive step, Specification, Types of patent application, process E-filing, Examination of patent, Grant of patent, Revocation, Equitable Assignments, Licenses, Licensing of related patents, patent agents, Registration of patent agents.

### Textbooks:

1. Research Methodology: A Step-by-Step Guide for Beginners, Ranjit Kumar, Sage Publications, 4<sup>th</sup> Edition, 2015.
2. Intellectual Property: A Very Short Introduction, Siva Vaidhyanathan, Oxford University Press, 2017.
3. Intellectual Property: The Law of Trademarks, Copyrights, Patents, and Trade Secrets" Deborah E. Bouchoux, Cengage India, 4<sup>th</sup> Edition, 2013.

### Reference Books:

1. Research methodology: an introduction for science & engineering students, Stuart Melville and Wayne Goddard, Juta Academic, 2<sup>nd</sup> Edition, 2014.
2. Research design: Qualitative, quantitative, and mixed methods approach, Creswell, J.W. and Creswell, J.D., Sage publications, 2017.
3. Intellectual Property in New Technological Age, Robert P. Merges, Peter S. Menell, Mark A. Lemley, Clause 8 Publishing; Volume I: Perspectives, Trade Secrets & Patents; 2023.

**Web Links:**

1. <https://archive.nptel.ac.in/courses/121/106/121106007/#>
2. [https://onlinecourses.swayam2.ac.in/ntr24\\_ed08/preview](https://onlinecourses.swayam2.ac.in/ntr24_ed08/preview)

## Research and Publication Ethics

**Course Code: 246UC004**

### **UNIT-I:**

#### **Philosophy & Ethics**

##### **Introduction to Philosophy:**

Definition, Nature & Scope, Concept, Branches

**Ethics:** Definition, Moral Philosophy, Nature of Moral Judgements & Reactions

### **UNIT-II:**

#### **Scientific Conducts**

Ethics with respect to Science and Research, Intellectual Honesty & Research Integrity

##### **Scientific Misconducts:**

Falsification, Fabrication & Plagiarism

##### **Redundant Publications:**

Duplicate & Overlapping Publication, Salami Slicing, Selective Reporting & Misrepresentation of Data

### **UNIT-III:**

#### **Publication Ethics:**

Definition, Introduction and Importance

##### **Best Practices/ Standard Setting Initiatives and Guidelines:**

COPE, WAVE, etc., Conflicts of Interest

##### **Publication Misconduct:**

Definition, Concept, Problems that lead to unethical behavior and vice versa, types, Violation of Publication Ethics, Authorship and Contributorship, Identification of Publication Misconduct, Complaints and Appeals, Predatory Publishers and Journals

### **UNIT-IV:**

#### **Open Access Publishing**

Open Access publications and Initiatives, SHERPA/ RoMEO online resource to check publisher copyright and self-achieving policies, Software tool to identify predatory publications developed by SPPU, Journal Finder/ Journal Suggestion tools viz. JANE, ELSEVIER, SPINGER, Journal suggester etc.

### **UNIT-V:**

#### **Publication Misconduct**

##### **A: Group Discussions:**

Subject-specific Ethical issues, FFP, Authorship, Conflicts of Interest, Complaints and Appeals: Examples and fraud from India and Abroad

##### **B: Software tools:**

Use of Plagiarism software like Turnitin, Urkund and other open source software tools

### **Unit-VI:**

#### **Database and Research Metrics**

##### **A: Database:**

Indexing database, Citation database: web of science, Scopus etc.

Impact factor of journal as per journal citation report, SNIP, SJR, IPP, cite score

**B. Metrics:** h-index, g-index, i-10 index, AL metrics etc.

**Textbooks:**

1. Philosophy in Science, Bird A, Routledge, 1<sup>st</sup> Editon, Roultedge, 2006.
2. A Short History of Ethics, MacIntyre, London, 1<sup>st</sup> Editon, Roultedge 1967.

**Reference Book:**

1. Ethics in Science, Education and Governance, Indian National Science Academy, 1<sup>st</sup> Editon, 2019.

**Web links:**

1. [www.niehs.nih.gov/research/resources/bioethics/whatis](http://www.niehs.nih.gov/research/resources/bioethics/whatis)
2. [https://onlinecourses.swayam2.ac.in/nou22\\_ge73/preview](https://onlinecourses.swayam2.ac.in/nou22_ge73/preview)

## Theoretical and Computational Chemistry-Methods and Applications

Course Code: 246CH001

### Unit-I:

#### Quantum Chemistry Fundamentals:

Introduction to Theoretical and Computational Chemistry: Overview of theoretical and computational chemistry. Historical development and significance in chemical research, Basic concepts: Quantum mechanics, molecular modeling, and simulation. Principles of quantum mechanics: Schrödinger equation, wavefunctions, and probability densities. Approximation methods: Hartree-Fock theory, Density Functional Theory (DFT), and post-Hartree-Fock methods. Basis sets and computational methods for solving the Schrödinger equation. Case studies: Applications of quantum chemistry in predicting molecular properties.

### Unit-II:

#### Software and Tools for Computational Chemistry:

Introduction to popular computational chemistry software: Gaussian, VASP, GAMESS, and others. Practical sessions: Hands-on experience with computational tools and software. Data analysis and visualization techniques in computational chemistry

### Unit-III:

#### Computational Methods for Reaction Dynamics:

Potential energy surfaces and reaction pathways. Transition state theory and saddle point search methods. Molecular dynamics simulations of chemical reactions, Case studies: Computational studies of reaction mechanisms and kinetics.

### Unit-IV:

#### Advanced Computational Techniques:

Multiscale modeling: Coupling quantum mechanics with molecular mechanics (QM/MM). Machine learning and data-driven approaches in computational chemistry, High-performance computing and parallel processing in chemical simulations, Case studies: Applications of advanced computational techniques in complex chemical systems

### Unit-V:

#### Critical Evaluation and Validation of Computational Results:

Comparing computational results with experimental data. Error analysis and uncertainty in computational predictions. Validation techniques: Benchmarking and cross-validation with experimental data.

### Textbooks:

1. "Molecular Quantum Mechanics" by Peter Atkins and Ronald Friedman, Oxford University Press, 5<sup>th</sup> Edition, 2010
2. "Introduction to Computational Chemistry" by Frank Jensen, Wiley 3<sup>rd</sup> Edition, 2017.
3. "Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems" by David C. Young, Wiley- Interscience, 2001.

**Reference Books:**

1. "Principles of Quantum Chemistry" by J. Robert Peterson and Barry A. Messer, 1<sup>st</sup> Edition, Prentice Hall, 1994.
2. "Molecular Modelling: Principles and Applications" by Andrew R. Leach, 2<sup>nd</sup> Edition, Pearson Education, 2001.

**Weblinks:**

1. <https://archive.nptel.ac.in/courses/104/101/104101095/>
2. <https://archive.nptel.ac.in/noc/courses/noc18/SEM2/noc18-cy13/>

## Interpretative Molecular Spectroscopy

Course Code: 246CH002

### Unit-I:

#### Spectroscopy Introduction

Introduction to spectroscopy, different types of spectroscopic methods, General Process for Structure Elucidation of an Unknown, Spectral Interpretation, brief discussion on all spectroscopic and analytical methods

### Unit-II:

#### Nuclear Magnetic Resonance Spectroscopy:

Introduction to NMR, Basic aspects, nuclear spin, magnetic field, shielding, NMR signals, NMR spectrometer, Proton NMR, NMR spectra of simple molecules, chemical shifts, coupling constants etc.

$^1\text{H}$  NMR:  $^1\text{H}$  NMR spectra of organic, inorganic and organometallic compounds, different types of couplings. Compounds with other NMR active nuclei such as  $^{11}\text{B}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  and their interactions and couplings, Analysis and interpretation of numerous examples

$^{13}\text{C}$  NMR, brief introduction, interpretation of  $^{13}\text{C}$  NMR spectra,  $^{31}\text{P}$  NMR, brief introduction, Interpretation and analysis of  $^{31}\text{P}$  NMR spectra of phosphorus compounds, phosphines, coordination compounds and organometallic compounds containing organophosphorus ligands, Studying reaction mechanisms using  $^1\text{H}$  and  $^{31}\text{P}$  NMR spectral data, Complex spectra containing several NMR active nuclei and understanding the splitting patterns Multinuclear NMR, Discussion on various NMR active nuclei other than  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{31}\text{P}$ , NMR spectra of compounds containing lithium, boron, silicon, selenium, tungsten, rhodium and platinum

### Unit-III:

#### Ultraviolet-Visible Spectroscopy (UV-Vis):

UV-visible spectroscopy: microstates, term symbols, determining ground term. Selection rules, Spin-orbit coupling, classification of d-d transitions. Orgel diagram, TS-diagram, Charge transfer transitions.

Interpretation of electronic spectra of coordination compounds,  $d^1$ — $d^9$  system, Examples for each system, Application of UV-visible spectroscopy in understanding inorganic reaction mechanism

### Unit-IV:

#### Infrared Spectroscopy (IR) & Mass Spectrometry (MS)

IR spectroscopy, Brief introduction, Interpretation of IR spectra of inorganic, organic and organometallic compounds,

Mass spectrometry: Brief introduction, fundamentals of mass spectrometry. Different methods, Data interpretation, Examples of inorganic, organic and organometallic compounds

### Unit-V:

#### Integration of Spectroscopic Techniques:

Summary, IR spectroscopy continued with more examples: Elucidation of structures using a combination of NMR, UV-visible and IR spectral data. Examples of inorganic, organic and organometallic compounds, other applications and summarizing all spectroscopic methods

**Textbooks:**

1. Inorganic Chemistry, 3rd Edition, D. F. Shriver, P. W. Atkins, Oxford University Press, Oxford, 1999.
2. Inorg. Chemistry 2<sup>nd</sup>, 3<sup>rd</sup> or 4<sup>th</sup> Edition, C. E. Housecroft and A. G. Sharpe, Pearson, Prentice Hall, 2008, 2012, 2018.
3. Nuclear Magnetic Resonance, W. W. Paudler, John Wiley & Sons, First Edition, 1987.

**Reference Books:**

1. Introduction to Multinuclear NMR, C. H. Yoder and C. D. Schaeffer Jr., Benjamin / Cummings, Pub, Co., First Edition, 1987.
2. Organic Spectroscopy, 3rd Ed. W. Kemp. Phosphorus-31, NMR spectroscopy, Olaf Kuhl, Springer, 2008.

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc25\\_ch19/preview](https://onlinecourses.nptel.ac.in/noc25_ch19/preview)
2. [https://onlinecourses.nptel.ac.in/noc22\\_cy45/preview](https://onlinecourses.nptel.ac.in/noc22_cy45/preview)

## **Advanced Organic Synthesis: Oxidation, Reduction, and C-C Bond Formation Strategies for Natural Product Synthesis**

**Course Code: 246CH003**

### **Unit I:**

#### **Organic Synthesis: Oxidation Methods and Applications of Sulfur and Selenium-Based Reagents**

Introduction to organic synthesis, importance of selectivity and basics of oxidation of alcohols and development of sulfur-based oxidations: Swern oxidation and related concepts, Continuation of Swern oxidation and the utility of intermediates derived from Swern oxidation including Pamperer intermediates, Oxidations using selenium compounds such as  $\text{SeO}_2$  and organo selenium compounds

### **Unit II:**

#### **Advanced Oxidation Techniques in Organic Synthesis: Hypervalent Iodine, Transition Metals, and Modern Reagents**

Dess-Martin, IBX and related hypervalent iodine-based oxidations, silver carbonate/celite, Prevost reactions and their modern variation. Microbial oxidations such as *Pseudomonas Putida* etc., Oxidations with  $\text{RuO}_4$  and other Transition metal catalyzed oxidations, Tamao-Fleming Oxidation. Oxidations with Dimethyl dioxirane (DMDO) and 2-sulfonyloxaziridines and chiral versions

### **Unit III:**

#### **Selective Oxidation and Reduction Strategies in Organic Synthesis: Modern Reagents and Techniques**

Oxidations at unfunctionalised carbons, Photosensitized oxidations, Reduction of Carbonyl compounds with Boron and Aluminium based reagents such as Luche Reduction,  $\text{NaCN}(\text{BH}_3)$ , DIBAL, Red-Al, L- and K- Select rides, Super hydrides and associated selectivity's, Low Valent Titanium species and Microbial reductions (NADH model etc.), Dissolving Metal Reductions Reduction with Silanes.

### **Unit IV:**

#### **Asymmetric Synthesis: Epoxidation, Dihydroxylation, Reductions, and C-C Bond Formation Strategies**

Sharpless epoxidation and synthetic utility of the chiral epoxy alcohols, Katsuki-Jacobsen epoxidation and mechanistic details,  $\text{OsO}_4$  based and related Sharpless Asymmetric Dihydroxylation, Corey's oxazaborolidines in asymmetric reductions, Noyori's Ruthenium catalyzed reduction of ketones, Asymmetric Hydrogenations with BINAP, C-C Bond formation via Carbanions alpha to electron withdrawing groups. Boron and Silicon Enolates: Formation and Use in C-C Bond Formation, Imines in C-C Bond Formation.

### **Unit V:**

#### **Advanced Methods in Organic Synthesis: Cyclopropanation, Chiral Ligands, and Natural Product Synthesis**

Simmons-Smith Cyclopropanation in Organic Synthesis, Use of Allyl Boron, Allyl and Vinyl

Silanes and Allyl Tin compounds in C-C Bond Formation, Introduction to SAMP and RAMP chiral ligands for asymmetric C-C bond formation, Introduction to Oppolzer's Sultam based chiral ligands and their reactions for organic synthesis, Evans' Oxazolidinone for asymmetric synthesis, Synthesis of selected natural products using above discussed methods of oxidation, reduction and C-C Bond formations, Synthesis of selected natural products using above discussed methods of oxidation, reduction and C-C Bond formations

**Text Books:**

1. Organic Synthesis by M.B. Smith, 4<sup>th</sup> Edition, Wiley, 2011.
2. Modern Synthetic Methods by W Carruthers, 1<sup>st</sup> Edition, Wiley, 1990

**Reference Books:**

1. Classics in Total Synthesis (Parts I-III) by K. C. Nicolaou, 1<sup>st</sup> Edition, 1996, 2000, 2004, Wiley-VCH.
2. Organic Mechanisms by R. Bruckner, 1<sup>st</sup> Edition, Wiley, 1993.

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc22\\_cy27/preview](https://onlinecourses.nptel.ac.in/noc22_cy27/preview)
2. <https://pubs.acs.org/doi/10.1021/acscentsci.0c00549>

## Chemistry of Nanomaterials

Course Code: 246CH004

### Unit I:

#### **Introduction to Nanoscience: Natural Systems, Size-Dependent Properties, and Synthesis Techniques**

Introduction to Nanoscience and Nanotechnology, Nano systems in Nature, Size Dependent Properties of Nanomaterials, Synthesis of Nanomaterials: The top-down Approach, Synthesis of nanomaterials: The bottom-up approach

### Unit II:

#### **Characterization Techniques for Nanomaterials: Principles, Methods, and Applications**

Characterization of nanomaterials - An overview, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), Photon Probe Characterization Methods, Energy dispersive X-ray Spectroscopy (EDAX) and Powder X-ray Diffraction, UV-Visible Spectroscopy-Bandgap determination, Application of IR-Spectroscopy

### Unit III:

#### **Advances in Nanomaterials: Metal Nanoparticles, Carbon-Based Nanostructures, and Polymer Nanocomposites**

Metal Nanoparticles, Surface Plasmon Resonance (SPR), Applications of Metal Nanoparticles, Alloy Nanoparticles, Metal Nanoclusters, Quantum Dots: Optical Properties and Applications, Carbon Based Nanomaterials-An Overview, Fullerenes: Properties and Applications, Carbon Nanotubes, Graphene and its Derivatives, Carbon Dots and other Carbon Nanostructures, Nanocomposites and Fibers, Polymer Based Nanomaterials

### Unit IV:

#### **Exploring Nanoscale Chemistry: MOFs, supra molecular Systems, and Functional Nanomaterials**

Metal organic Frame works (MOF), Chemical Interactions at the Nanoscale, supra molecular Chemistry, Luminescent Nanomaterials, Magnetism in Nanomaterials, Applications of luminescent and Magnetic Nanomaterials, Biological Nanomaterials

### Unit V:

#### **Applications and Innovations in Nanotechnology: Nanoelectronics, Sensors, Catalysis, and Biomedicine**

Nanoelectronics, Nanosensors, Nanocatalysis, Biocompatible Nanomaterials, Diagnostic and Therapeutic Applications of Nanomaterials, Nanomaterial Research in India

### Text Books:

1. Rao, C.N.R., & Matte, H.S.S.R, Nanomaterials chemistry: Recent developments and new directions, 1<sup>st</sup> Edition, Wiley-VCH.
2. Edelstein, A.S., & Cammarata, R.C. (2001). Nanomaterials: Synthesis, properties, and applications. CRC Press, 1<sup>st</sup> edition, 2001.
3. Rao, C.N.R., & Müller, A. (2003). Nanomaterials chemistry: A review of the scientific and technological aspects. World Scientific 1<sup>st</sup> Edition.

4. Vollath, D. (2008). Nanomaterials: Synthesis, characterization, and applications, 1<sup>st</sup> Edition, Wiley-VCH.

**Reference Books:**

1. Haghi, A.K., & Zaikov, G.E. (2014). Nanomaterials: Science and Applications. Apple Academic Press.
2. Poole, C.P., & Owens, F.J. (2003). Introduction to nanotechnology. Wiley.
3. Cao, G. (2004). Nanostructures & nanomaterials: Synthesis, properties & applications. Imperial College Press.
4. Hornyak, G.L., Tibbals, H.F., Dutta, J., & Moore, J.J. (2008). Introduction to Nanoscience and Nanotechnology. CRC Press

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc21\\_mm38/preview](https://onlinecourses.nptel.ac.in/noc21_mm38/preview)
2. [https://onlinecourses.nptel.ac.in/noc24\\_me80/preview](https://onlinecourses.nptel.ac.in/noc24_me80/preview)

## **Nuclear Chemistry in Research and Industry-Techniques and Innovations**

**Course Code: 246CH005**

### **Unit-I:**

#### **Fundamentals of Nuclear Chemistry:**

Introduction to Nuclear Chemistry: Basic concepts of nuclear structure, nuclear forces, and stability. Nuclear reactions: Fission, fusion, and radioactive decay. Types of radioactive decay: Alpha, beta, and gamma emissions. Nuclear Models: Liquid drop model, shell model, and collective model. Magic numbers and nuclear spin. Energy levels and nuclear spectroscopy

### **Unit-II:**

#### **Radioactivity and Radiochemistry:**

Radioactive Decay Kinetics: Decay laws, half-life, and mean life. Radioactive series and secular equilibrium. Detection and measurement of radioactivity. Radiochemistry Techniques: Separation techniques in radiochemistry. Radiochemical purity and isotopic labelling. Radiotracers in chemical and biological systems.

### **Unit-III:**

#### **Nuclear Reactions and Applications:**

Nuclear Reaction Mechanisms: Types of nuclear reactions: Elastic and inelastic scattering, capture reactions. Cross-sections and reaction rate calculations. Compound nucleus and direct reactions. Applications in Energy Production: Nuclear reactors: Types, design, and operation. Nuclear fuel cycle: Mining, enrichment, and waste management. Nuclear fusion: Principles and potential as an energy.

### **Unit-IV:**

#### **Analytical Techniques in Nuclear Chemistry:**

Radiation Detection and Measurement: Gas ionization detectors, scintillation detectors, and semiconductor detectors. Gamma spectroscopy, alpha spectroscopy, and neutron activation analysis. Dosimetry and radiation safety protocols. Nuclear Analytical Methods: Isotope dilution analysis, neutron activation analysis, and gamma-ray spectrometry. Applications in environmental monitoring, materials science, and medicine. Innovations in radiation detection technologies.

### **Unit-V:**

#### **Environmental and Safety Considerations:**

Environmental Impact of Nuclear Technologies: Radioactive waste management and disposal. Environmental monitoring of nuclear facilities. Radiation protection and regulatory standards. Safety in Nuclear Chemistry: Radiation hazards and safety protocols. Emergency preparedness and response to nuclear incidents. Ethics and public perception of nuclear technology.

### **Text Books:**

1. Radiochemistry and Nuclear Chemistry, Gregory Choppin, Jan-Olov Liljenzin, Jan Rydberg, 3<sup>rd</sup> Edition, Elsevier, 2013.

2. Nuclear and Radiochemistry: Fundamentals and Applications, Karl Heinrich Lieser, 1<sup>st</sup> edition, Wiley- VCH, 2001.
3. Introduction to Nuclear Chemistry, Harold C. Beard, 1<sup>st</sup> Edition, Prentice Hall, 1969.

**Reference Books:**

1. Fundamentals of Radiation Chemistry, A. Mozumder, Y. Hatano. 1<sup>st</sup> edition, CRC press, 2002.

**Weblinks:**

1. <https://archive.nptel.ac.in/courses/104/101/104101137/>
2. <https://nptel.ac.in/courses/115102017>

## Sensor Technologies in Chemistry-Principles and Applications

Course Code: 246CH006

### Unit-I:

#### Introduction to Sensor Technologies:

Principles of Chemical Sensing: Basic concepts and definitions. General principles of sensor operation. Sensor performance metrics: Sensitivity, selectivity, limit of detection, and response time. Classification of Sensors: Electrochemical sensors: Amperometric, potentiometric, and conductometric sensors. Optical sensors: Absorbance, fluorescence, and surface plasmon resonance sensors. Biosensors: Enzyme-based, immuno-sensors, and nucleic acid sensors. Sensor Design and Fabrication: Design considerations for sensor materials and structures. Fabrication techniques: Lithography, deposition, and microfabrication. Integration of sensors with electronic and data acquisition systems.

### Unit-II:

#### Electrochemical Sensors:

Fundamentals of Electrochemical Sensing: Electrochemical cell components and functions. Electrode reactions and mechanisms. Types of electrochemical sensors: Potentiometric, amperometric, and conductometric. Applications and Case Studies: Environmental monitoring: Detection of pollutants and gases. Clinical diagnostics: Blood glucose sensors and clinical analytes. Industrial applications: Process control and quality assurance. Advanced Electrochemical Sensors: Nanomaterial-based sensors: Carbon nanotubes, graphene, and metal nanoparticles. Flexible and wearable sensors: Design and applications.

### Unit-III:

#### Optical Sensors:

Principles of Optical Sensing: Interaction of light with matter: Absorption, fluorescence, and scattering. Optical transduction mechanisms: Surface plasmon resonance (SPR), interferometry, and resonant scattering. Types of Optical Sensors: Absorbance-based sensors: UV-Vis and NIR spectroscopy. Fluorescence sensors: Fluorimetry and luminescence. Surface plasmon resonance (SPR) sensors: Principles and applications. Applications and Case Studies: Environmental monitoring: Detection of water contaminants and pollutants. Biomedical applications: Cellular imaging and diagnostics. Industrial processes: Quality control and product analysis.

### Unit-IV:

#### Biosensors:

Introduction to Biosensors: Components of biosensors: Bioreceptor, transducer, and signal processor. Types of biosensors: Enzyme-based, immuno-sensors, and nucleic acid sensors. Mechanisms of Biosensing: Enzyme-based sensors: Mechanism and applications. Immuno-sensors: Antibody-antigen interactions and detection methods. Nucleic acid sensors: DNA/RNA detection and molecular diagnostics. Applications and Case Studies: Medical diagnostics: Point-of-care testing and personalized medicine. Environmental monitoring: Detection of biological contaminants. Food safety: Detection of pathogens and allergens.

## **Unit-V:**

### **Advanced Sensor Technologies:**

Design and Fabrication of Nanosensors: Techniques for integrating nanomaterials into sensor devices. Nanoscale fabrication methods: Lithography, self-assembly, and chemical vapor deposition. Examples of Nanosensors designs for various applications. Biological and Medical Nanosensors: Nanosensors in medical diagnostics: Biosensors for detecting biomolecules and pathogens. Role of nanotechnology in personalized medicine and health monitoring. Case studies: Glucose Nanosensors, cancer detection Nanosensors, and wearable Nanosensors.

### **Textbooks:**

1. Robert W. Cattrall, Chemical Sensors, Oxford Chemistry Primers, Oxford Science Publications, 1<sup>st</sup> edition, 1997.
2. C.M.A. Brett and A.M.O. Brett, Electroanalysis, Oxford Chemistry Primers, Oxford Science Publications, 1<sup>st</sup> Edition, 1988.
3. J. Janata, 1989, 1<sup>st</sup> Edition, Principles of Chemical Sensors, Plenum Press, New York.

### **Reference Books:**

1. T. E. Edmonds (ed.), 1988, 1<sup>st</sup> Edition, Chemical Sensors, Chapman and Hall, New York
2. C. Alexander et al, 19, 106, Journal of Molecular Recognition (a review article), 2006.

### **Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc23\\_ee95/preview](https://onlinecourses.nptel.ac.in/noc23_ee95/preview)
2. [https://onlinecourses.nptel.ac.in/noc24\\_ce71/preview](https://onlinecourses.nptel.ac.in/noc24_ce71/preview)

## Organic Transformations and Reagents-Catalysis, Selectivity, and Functional Group Interconversions

Course Code: 246CH007

### Unit-I:

#### Oxidations and oxidizing reagents:

Overview of organic transformations; importance of functional group inter conversion in synthesis. Functional Group Interconversions: Common interconversions include oxidation, reduction, hydrolysis, and protection / deprotection strategies. Introduction, Definition, and Types of Oxidations: Introduction, preparation methods, properties, and synthetic applications of DDQ, SeO<sub>2</sub>, NBS, peracids, Prevost dihydroxylation, Woodward's modified dihydroxylation, chromium (VI) oxidants, KMnO<sub>4</sub>, OsO<sub>4</sub>, MnO<sub>2</sub>, Ag<sub>2</sub>CO<sub>3</sub>, Pb(OAc)<sub>4</sub>, and HIO<sub>4</sub>. Epoxidation and Epoxidation Reagents

### Unit-II:

#### Reductions and Reducing Reagents:

Introduction, definition, and types of reductions. Introduction, preparation methods, properties, and synthetic applications of Hydride Transfer Reagents LiAlH<sub>4</sub> and its derivatives, NaBH<sub>4</sub> and its derivatives, Metal-Based Reductions: Using Li, Na, Ca in liquid ammonia; sodium, magnesium, zinc, titanium, and samarium (e.g., Birch reduction, pinacol formation, McMurry coupling, acyloin formation, dehalogenation, and deoxygenation). Catalytic Hydrogenation: Heterogeneous (palladium, platinum, rhodium, nickel) and homogeneous (Wilkinson's catalyst). Transfer Hydrogenation and Noyori Asymmetric Hydrogenation.

### Unit-III:

#### Organometallics and Organometallic reagents:

Introduction, Definition, and Types of Organometallics; Introduction, preparation methods, types, properties, and synthetic applications of Organolithium reagents, Organomagnesium reagents, Organocopper reagents, Organoboron reagents, Organosilicon reagents, Organostin reagents, and Organopalladium reagents (Coupling reactions).

### Unit-IV:

#### Chemo-, Regio-, and Stereoselective Transformations:

Chemo- and Regioselectivity: Principles of chemo selectivity: Protecting groups and selective functionalization. Regioselectivity in aromatic substitution, electrophilic addition, and cyclization reactions. Stereoselective Transformations: Principles of stereoselectivity: Stereoselective vs. stereospecific reactions. Asymmetric synthesis: Chiral auxiliaries, catalysts, and reagents. Enantioselective catalysis: Sharpless epoxidation, CBS reduction, and asymmetric hydrogenation. Applications and Case Studies: Designing stereoselective routes in complex organic synthesis. Recent advances in chemo-, regio-, and stereoselective methodologies.

### Unit-V:

#### Complex Molecule Synthesis:

Application of organic transformations in total synthesis. Designing synthetic routes with selectivity considerations. Industrial and Pharmaceutical Applications: Catalytic processes in drug synthesis. Case studies: Industrial scale organic transformations and reagent use.

**Textbooks:**

1. Francis A. Carey and Richard J. Sundberg (Part A: Structure and Mechanisms), University of Virginia, Charlottesville, Virginia, 5<sup>th</sup> Edition, Springer, 2007
2. Francis A. Carey and Richard J. Sundberg (Part B: Reactions and Synthesis), University of Virginia, Charlottesville, Virginia, 5<sup>th</sup> Edition, Springer, 2007.
3. "Organic Chemistry" by R. T. Morrison and R. N. Boyd (Prentice Hall), 6<sup>th</sup> Edition, Prentice Hall, 1992.

**Reference Books:**

1. Modern Organic Synthesis: An Introduction, George S. Zweifel and Michael He Nantz, University of California, 1<sup>st</sup> Edition, Wiley, 2007,
2. W. Carruthers and Iain Coldham, "Modern Methods of Organic Synthesis," Cambridge University Press, 4<sup>th</sup> Edition, 2004.

**Weblinks:**

1. <https://archive.nptel.ac.in/courses/104/103/104103023/>
2. <https://archive.nptel.ac.in/courses/104/105/104105032/>

## Medicinal Chemistry

Course Code: 246CH008

### Unit I:

#### Fundamentals of Drug Action and Targets

An overview of drugs and drug targets; structure of a cell; intermolecular binding forces; classification of drugs

### Unit II:

#### Enzyme Structure, Catalysis, and Inhibition in Drug Discovery

Principles of enzyme structure, catalysis and inhibition in drug discovery, reversible and irreversible inhibitors; transition-state inhibitors; case studies

Receptor's function and ligand binding interactions; Ion channel receptors; kinase-linked receptors; G-Protein coupled receptors, drug-receptor interaction; dose-response curves; case studies

### Unit III:

#### Nucleic Acids and Chemotherapy Agents

Nucleic acids structure and function; DNA Interactive agents and chemotherapy: DNA binding agents; intercalation and alkylation; DNA strand breakers; case studies

### Unit IV:

#### Drug Discovery, Design, and Optimization

Synthetic methods in medicinal chemistry: Combinatorial and parallel synthesis: solid phase techniques, mix and split method in combinatorial synthesis; dynamic combinatorial synthesis; solid phase synthesis; diversity-oriented synthesis.

Lead discovery; Bioassays; drug targets; Lead Modification; optimization; pharmacophore; homology; bioisostere; chain branching; Electronic effects; Lipophilicity; Structure-Activity Relationships; Quantitative-structure activity relationships (QSAR).

### Unit V:

#### Drug Metabolism, Delivery, and Resistance

Drug metabolism and pharmacology: Analytical methods in metabolism; Phase I and Phase II transformations; Absorption, distribution, metabolism and excretion (ADME); bioavailability; pre-clinical and clinical development; therapeutic index and therapeutic window.

Prodrugs and drug delivery systems: Use of prodrug systems; prodrugs for stability, solubility and slow release; overview of drug delivery

Drug resistance mechanisms and synergisms: Mechanisms of drug resistance; circumventing drug resistance; drug synergy

### Textbooks:

1. An Introduction to Medicinal Chemistry, Graham L. Patrick; 2<sup>nd</sup> Edition, Oxford University Press, 2001.
2. The Organic Chemistry of Drug Design and Drug Action, Richard B. Silverman, Second Edition Lehninger's Principles of Biochemistry, Cox and Nelson, Fifth Edition 2<sup>nd</sup> Edition, Elsevier, 2004.
3. "Catalytic Asymmetric Synthesis" by Iwao Ojima, 1<sup>st</sup> edition, Wiley – VCH, 2000.

**Reference Books:**

1. Lehninger's Principles of Biochemistry, Cox and Nelson, 5<sup>th</sup> Edition, WH Freeman & Co, 2008.
2. Foye, W. O., Lemke, T. L., & Williams, D. A. (2019). Foye's Principles of Medicinal Chemistry (8th Ed.). Wolters Kluwer Health.

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc25\\_cy22/preview](https://onlinecourses.nptel.ac.in/noc25_cy22/preview)
2. [https://onlinecourses.nptel.ac.in/noc20\\_cy16/preview](https://onlinecourses.nptel.ac.in/noc20_cy16/preview)

## **Advanced Green Chemistry-Sustainable Strategies and Innovations in Chemical Processes**

**Course Code: 246CH009**

### **Unit-I:**

#### **Introduction, Metrics and Assessment in Green Chemistry:**

Introduction to Green Chemistry: Definition, Evolution, and Importance of Green Chemistry. The 12 Principles of Green Chemistry and their practical applications. Relationship between green chemistry, sustainability, and environmental policy. Case studies on successful applications of green chemistry in industry. Key metrics in evaluating green chemistry: Atom economy, E-factor, and process mass intensity (PMI). Life cycle assessment (LCA) of chemical products and processes. Environmental, economic, and social dimensions of sustainability in chemical industries. Tools for measuring sustainability in chemical reactions and processes. Comparative analysis of traditional versus green processes using green chemistry metrics

### **Unit-II:**

#### **Catalysis, Solvent-Free Reactions and Green Solvents in Green Chemistry:**

Role of catalysts in green chemistry: Homogeneous, heterogeneous, and biocatalysis. Design of recyclable, efficient, and selective catalytic processes. Applications of organocatalysis, enzymatic catalysis, and photocatalysis in sustainable chemistry. Case studies: Green catalytic processes in industrial applications. Environmental and economic concerns with traditional solvents. Alternatives to hazardous solvents: Supercritical fluids, ionic liquids, deep eutectic solvents, and water as a solvent. Solvent-free synthesis and its advantages in green chemistry. Green solvent selection criteria and case studies of green solvent use in industrial processes.

### **Unit-III:**

#### **Environmental Remediation in Green Chemistry:**

Use of green chemistry in environmental remediation and pollution control. Green techniques for wastewater treatment, heavy metal removal, and air purification. Nanomaterials and green catalysts for environmental cleanup, Case studies: Green chemistry solutions for environmental challenges.

### **Unit-IV:**

#### **Innovations in Green Chemistry:**

Cutting-edge innovations in green chemistry for sustainable practices. Green chemistry approaches pharmaceuticals, agrochemicals, and materials science. Case studies: Breakthrough innovations in green synthesis and process design. Research trends and future directions in green chemistry

### **Unit-V:**

#### **Regulatory Frameworks and Policies for Green Chemistry:**

Global regulatory frameworks promoting sustainable chemistry (REACH, TSCA, etc.). Incentives for adopting green chemistry practices in industry. Role of government, academia, and industry in promoting green chemistry. Ethical and societal impacts of green chemistry in the modern world

**Textbooks:**

1. Green Chemistry: Theory and Practice, Paul T. Anastas and John C. Warner, 1<sup>st</sup> Edition, Oxford University Press, 1998.
2. Introduction to Green Chemistry, Albert S. Matlack, 1<sup>st</sup> Edition, Marcel Dekker, 2001.
3. Sustainable Industrial Chemistry: Tools and Principles, Fabrizio Cavani, Gabriele Centi, and Siglinda Perathoner, 1<sup>st</sup> Edition, Wiley-VCH, 2014.

**Reference Books:**

1. Green Chemistry and Engineering: A Practical Design Approach, Concepción Jiménez-González and David J. C. Constable, 1<sup>st</sup> Edition, Wiley-Interscience, 2009.
2. Green Solvents for Chemistry: Perspectives and Practice, William M. Nelson, 1<sup>st</sup> Edition, Wiley, 2013.

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc21\\_mg85/previ](https://onlinecourses.nptel.ac.in/noc21_mg85/previ)
2. [https://onlinecourses.nptel.ac.in/noc23\\_ge17/preview](https://onlinecourses.nptel.ac.in/noc23_ge17/preview)

## **Environmental Quality Monitoring & Analysis**

**Course Code: 2246CH010**

### **Unit I:**

#### **Understanding Environmental Fate and Transport of Chemicals: Impacts, Mechanisms, and Health Risks**

Introduction; Definition of Environment; Link between source/environment/receptor; Exposure; Health effects; Toxicology; Defining the need for fate and transport. Chemicals of concern; relevant properties for environmental fate and transport; Definition of Equilibrium – partition constants, solubility, vapor pressure, Henry's constant,  $K_{oc}$ ,  $K_{ow}$  etc. Equilibrium partitioning of chemicals between different phases of the environment

### **Unit II:**

#### **Environmental Monitoring and Quality Control: Key Parameters, Methods, and Pollutant Assessment**

Parameters for environmental water/ air / soil / sediment – screening parameters, priority air pollutants – definitions of PM. Monitoring of environmental parameters – screening parameters – BOD, COD, TOC, TDS; Environmental sampling – definition and synthesis of a monitoring / sampling / analysis method. Quality Assurance and quality control (QA/QC).

Methods for sampling / processing / analysis of organic and inorganic constituents in air / water / soil / sediment

### **Unit III:**

#### **Modeling Environmental Transport and Atmospheric Dispersion: BOX Models and Gaussian Dispersion**

Introduction to environmental transport – BOX Models and the application to multimedia transport of pollutants, Atmospheric Dispersion – Gaussian Dispersion model

### **Unit IV:**

#### **Fundamentals of Mass Transport: Diffusion, Convection, and Inter-phase Chemical Flux**

Fundamentals of mass transport – definition of interphase and inter-phase chemical flux; Interphase mass transport, diffusion coefficient and convection mass transfer coefficients.

### **Unit V:**

#### **Mechanisms and Dynamics of Chemical Exchange in Environmental Interfaces**

Chemical Exchange between air-water, Chemical Exchange between sediment-water, Chemical exchange between soil-air, Overall transport model and scenarios

### **Textbooks:**

1. Environmental Chemodynamics - Louis J Thibodeaux, 2<sup>nd</sup> Edition, Wiley-Inter science, 2009.
2. Environmental Engineering – Peavy, Rowe and Tchobanoglous, 1<sup>st</sup> Edition, McGraw-Hill, 1985.

**Reference Books:**

1. Atmospheric Chemistry and Physics – Seinfeld and Pandis, 2<sup>nd</sup> Edition, Wiley-Interscience, 2006.

**Weblinks:**

1. [https://onlinecourses.nptel.ac.in/noc21\\_ch13/preview](https://onlinecourses.nptel.ac.in/noc21_ch13/preview)
2. [https://onlinecourses.nptel.ac.in/noc24\\_ag06/preview](https://onlinecourses.nptel.ac.in/noc24_ag06/preview)

## Industrial Wastewater Treatment

Course Code: 246CH011

### Unit I:

#### **Industrial Wastewater: Sources, Characteristics, Environmental Impact, and Treatment Methods**

Sources and characteristics of industrial wastewater & effect on environment, Management-volume reduction, neutralization, equalization and proportioning (SKG), Adsorption Process (SKG) & Ion Exchange Process (AS), Gas transfer & Air Stripping (Ammonia removal) (SKG)

### Unit II:

#### **Advanced Wastewater Treatment Technologies and Sustainable Disposal Practices**

Advanced Oxidation Processes (AS), Membrane processes for wastewater treatment (AS), Coagulation, Precipitation and Heavy Metal Removal (AS), Treatment and disposal of sludge (SKG) & Industrial Complexing for Zero Pollution Attainment (AS)

### Unit III:

#### **Industry-Specific Wastewater Treatment: Distillery, Dairy, Tannery, and Pulp & Paper Effluents**

Treatment of wastewater produced from Distillery and Dairy Industries (SKG), Treatment of wastewater produced from Tannery and Pulp and Paper (AS)

### Unit IV:

#### **Wastewater Treatment in the Textile, Dye, Fertilizer, Refinery, and Iron & Steel Industries**

Treatment of wastewater produced from Textile and Dye and Fertilizers (AS), Treatment of wastewater produced from Refineries and Iron & Steel (Coke Ovens) (SKG)

### Unit V:

#### **Wastewater Treatment in the Pharmaceutical and Mining Industries: Addressing Acid Mine Drainage and Industrial Effluents**

Treatment of wastewater produced from pharmaceutical industry. (AS), Mine Wastewater including Acid Mine Drainage (Coal mines, Washeries and coke oven plants) (SKG)

### Textbooks:

1. Environmental Engineering, S.K. Garg, 1<sup>st</sup> Edition, Khanna Publishers, 2004.
2. Water and Wastewater Technology, Mark J. Hammer and Mark J. Hammer Jr., 6<sup>th</sup> Edition, Prentice Hall, 2008.

### Reference Books:

1. Industrial Wastewater Treatment, A.D. Patwardhan, 1<sup>st</sup> Edition, Narosa Publishing House, 2001.

### Weblinks:

1. [https://onlinecourses.nptel.ac.in/noc25\\_ce33/preview](https://onlinecourses.nptel.ac.in/noc25_ce33/preview).
2. [https://onlinecourses.nptel.ac.in/noc24\\_ce105/preview](https://onlinecourses.nptel.ac.in/noc24_ce105/preview)

## Spectroscopy for Structural Elucidation

**Course Code: 246CH012**

### **Unit-I:**

Introduction to spectroscopic methods, UV-Vis spectroscopy, electronic transitions in organic molecules, selection rules, application of Beer Lambert law, qualitative and quantitative analysis by UV-Vis spectroscopy.

### **Unit-II:**

Infra-red spectroscopy – basic concepts, experimental methods, functional group analysis and identification using IR spectroscopy, structural effects on vibrational frequency.

### **Unit-III:**

Nuclear magnetic resonance spectroscopy (NMR), spin  $\frac{1}{2}$  nuclei,  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectroscopy, FT-NMR method. Chemical shifts, spin-spin coupling, spin-spin splitting pattern recognition for structure elucidation, coupling constants.  $^1\text{H}$  NMR spectroscopy, Second order effects in NMR spectrum, AB and AA'BB', ABC spin systems. Solving simple structure elucidation problems with  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy.

### **Unit-IV:**

Mass Spectrometry – various ionization methods – EI, CI, ESI and MALDI methods, fragmentation patterns of simple organic molecules, Use of HRMS. Fragmentation patterns of simple organic molecules (continued), solving structure elucidation problems using mass spectrometry.

### **Unit-V:**

Solving structure elucidation problems using multiple spectroscopic data (NMR, MS, IR and UV-Vis).

### **Textbooks:**

1. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, Herald Gunther, 3rd Edition, Kindle Edition, 2013
2. NMR Spectroscopy: A Physicochemical View, Harris, R. K., Pitman Publishing, 1986.

### **Reference Books:**

1. Introduction to Spectroscopy, Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R. (2015). (5th ed.). Cengage Learning
2. Spectrometric Identification of Organic Compounds, Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2015). (8th ed.). Wiley.

### **Web Links:**

1. [nptel.ac.in/courses/104106122](https://nptel.ac.in/courses/104106122)
2. [nptel.ac.in/courses/104106075](https://nptel.ac.in/courses/104106075)

## Reagents in Organic Synthesis

Course Code: 246CH013

### Unit I

#### Oxidizing Agents in Organic Transformations

**DDQ** – Mechanism and applications in dehydrogenation,

**Prevost and Woodward Hydroxylation** – Mechanistic comparison and synthetic applications,

**Chromium-Based Oxidizing Agents** – Jones reagent, PCC, PDC, etc.,

**Sulfur-Based Oxidizing Agents** – DMSO-based oxidations (Swern, Pfitzner–Moffatt, etc.),

**Miscellaneous Oxidants** – Silver carbonate, sodium periodate, lead tetraacetate, osmium tetroxide

### Unit II

#### Reducing Agents in Organic Transformations

**Part I - Hydride-based Reductions:** Lithium Aluminium Hydride ( $\text{LiAlH}_4$ ), Lithium Alkoxy Aluminium Hydride (L-Selectride, etc.), Sodium Borohydride ( $\text{NaBH}_4$ ), Red-Al (Sodium bis(2-methoxyethoxy) aluminium hydride), Borane-DMS, Diborane, 9-BBN, Meerwein–Ponndorf–Verley (MPV) Reduction

**Part II - Selective and Chemoselective Reductions:** Catalytic hydrogenation using Pd/C, Raney Nickel, Clemmensen Reduction, Wolff–Kishner Reduction

### Unit III

#### Non-Transition Metal Reagents in Organic Synthesis

**Grignard Reagents** – Nucleophilic addition and carbon–carbon bond formation

**Alkyl Lithium Reagents** – Structure, reactivity, selectivity

**Alkyl Boranes** – Hydroboration-oxidation and Suzuki coupling (intro)

**Iodine-Based Reagents** – Iodine monochloride, NIS, Iodine-mediated oxidations

### Unit IV

#### Organic Transformations Using Transition Metal Reagents

##### Part I – Palladium and Platinum:

Palladium-Catalyzed Cross-Coupling: Suzuki, Heck, Stille, Sonogashira, Platinum Catalyzed Reactions

##### Part II – Ruthenium, Iron, Osmium:

Ruthenium-Based Oxidations and Metathesis, Iron Catalyzed Reductions and Functionalizations, Osmium Tetroxide-Based Dihydroxylation

##### Part III – Gold-Catalyzed Transformations:

Electrophilic activation of alkynes and rearrangement reactions

### UNIT V

#### Organic Transformations Using Lanthanide Reagents

**Cerium (III) Chloride** – Chemoselective reductions, organocerium compounds

**Lanthanide Triflates** – Lewis acid catalysis in organic synthesis

**Applications in green chemistry and total synthesis**

**Textbooks:**

1. P. Wyatt and S. Warren, Organic Synthesis Strategy and Control, Wiley, 2007.
2. J. J. Li, Name Reaction, Springer, 2nd Edition, 2003

**Reference Books:**

1. Lanthanides in Organic Synthesis, T. Imamoto, Academic Press, 1994
2. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge, 4th Edition, 2015.
3. J. Clayden, Organic Chemistry, Oxford. 2nd Edition, 2014

**Web Links:**

1. [nptel.ac.in/courses/104103023](https://nptel.ac.in/courses/104103023)
2. [Molecular Rearrangements and Reactive Intermediates in Organic Synthesis - Course](#)

## Separation Techniques and Bioanalytical Chemistry

**Course Code: 246CH014**

### **Unit-I:**

Principle, theory, and applications of ultra-performance liquid chromatography (UPLC), hydrophilic interaction liquid chromatography (HILIC), preparative high-performance liquid chromatography, flash chromatography, counter current chromatography, chiral chromatography, size/molecular exclusion/gel permeation chromatography and affinity chromatography, multidimensional liquid chromatography.

### **Unit-II:**

Principle & theory, types of gas chromatography (GC) columns: packed and capillary columns, stationary phases-the key to different separations, temperature programming and carrier gas, types of sample injection, types of detectors: thermal conductivity, flame ionization, electron capture, flame photometric, flame thermionic and sulfur chemiluminescence detectors. Head space GC, pyrolysis GC, application in pharmaceutical, food, flavors, and fragrances analysis, multidimensional gas chromatography.

### **Unit-III:**

Theory & historical development of supercritical fluid chromatography (SFC), carbon dioxide as the mobile phase, column selection, mobile phase additives & modifiers, effect of temperature & pressure, instrumentation for analytical and preparative SFC, Chiral & achiral SFC, applications in pharmaceuticals, food analysis and natural products.

### **Unit-IV:**

Quantitative bioanalytical method development: extraction from biological matrices, importance of internal standards, chromatography, and detection systems. Bioanalytical method validation parameters: sensitivity, selectivity, accuracy and precision, linearity (calibration curves), recovery, matrix effect, stability, dilution reliability, ruggedness.

### **Unit-V:**

Bioavailability and bioequivalence study, incurred sample reanalysis test for subject samples. US Food and Drug Administration (FDA) guidance for bioanalytical method validation, acceptance criterion.

### **Text Books:**

1. "Principles and Practice of Bioanalysis" – Richard F. Venn (Taylor & Francis, 2008).
2. "Introduction to Modern Liquid Chromatography" – Lloyd R. Snyder, Joseph J. Kirkland, John W. Dolan (Wiley, 2010).

### **Reference Books:**

1. "Chromatographic Analysis of Pharmaceuticals" – John A. Adamovics (Marcel Dekker, 1997).
2. "Bioanalytical Chemistry" – Susan R. Mikkelsen & Eduardo Cortón (Wiley, 2016).
3. "Supercritical Fluid Chromatography: Fundamentals and Applications" – Gerald M. Randolph & Eric J. Levy (Elsevier).

**Web links:**

1. <https://nptel.ac.in/courses/103108100>
2. <https://nptel.ac.in/courses/103105060>