ADITYA UNIVERSITY

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
Total			**12**

Table 2: List of Domain-Specific Courses

List of Program Elective - 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	Essentials of Oxidation, Reduction, and C-C Bond Formation. Application in Organic 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

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-filling, 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, 4th 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, 4th Edition, 2013.

Reference Books:

1. Research methodology: an introduction for science & engineering students, Stuart Melville and Wayne Goddard, Juta Academic, 2nd 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

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
Publication Ethics: Definition, Introduction and Importance
Best Practices/ Standard Setting Initiatives and Guidelines: COPE, WAVE, etc., Conflictsof Interest
Publication Misconduct: Definition, Concept, Problems that lead to unethical behaviour 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
Group Discussions:
Subject-specific Ethical issues, FFP, Authorship, Conflicts of Interest, Complaints and Appeals: Examples and fraud from India and Abroad
Software tools:
Use of Plagiarism software like Turnitin, Urkund and other open source software tools
Database and Research Metrics:
Database:
Indexing database, Citation database: web of science, Scopus etc.
Impact factor of journal as per journal citation report, SNIP, SJR, IPP, cite score
Metrics: h-index, g-index, i-10 index, AL metrics etc.

Text Books:
1. Philosophy in Science, Bird A, Routledge, 2006.
2. A Short History of Ethics, MacIntyre, London, 1967.

Reference Book:
1. Ethics in Science, Education and Governance, Indian National Science Academy, 2019.

Weblinks:

1. www.niehs.nih.gov/research/resources/bioethics/whatis
2. 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, 5th Edition, 2010
2. "Introduction to Computational Chemistry" by Frank Jensen, Wiley 3rd Editon, 2017.
3. "Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems" by David C. Young, Wiley- Inter Science, 2001.

Reference Books:

1. "Principles of Quantum Chemistry" by J. Robert Peterson and Barry A. Messer, 1st Edition, Prentice Hall, 1994.

2. "Molecular Modelling: Principles and Applications" by Andrew R. Leach, 2nd 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}H NMR: ^{1}H NMR spectra of organic, inorganic and organometallic compounds, different types of couplings. Compounds with other NMR active nuclei such as ^{11}B, ^{19}F, ^{31}P and their interactions and couplings, Analysis and interpretation of numerous examples
^{13}CNMR, brief introduction, interpretation of ^{13}C NMR spectra, ^{31}P NMR, brief introduction, Interpretation and analysis of ^{31}P NMR spectra of phosphorus compounds, phosphines, coordination compounds and organometallic compounds containing organophosphorus ligands, Studying reaction mechanisms using ^{1}H and ^{31}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}H, ^{13}C and ^{31}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 2nd, 3rd or 4th Edition, C. E. Housecroft and A. G. sharpe, Pearson, Prentice Hall, 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., Benzamin / 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
2. https://onlinecourses.nptel.ac.in/noc22_cy45/preview

Essentials of Oxidation, Reduction, and C-C Bond Formation. Application in Organic 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 SeO2 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 RuO4 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, NaCN (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, OsO4 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, 4th Edition, Wiley, 2011.
2. Modern Synthetic Methods by W Carruthers, 1st Edition, Wiley, 1990

Reference Books:

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

Weblinks:

1. 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

Textbooks:

1. Rao, C.N.R., & Matte, H.S.S.R, Nanomaterials chemistry: Recent developments and new directions, 1st Edition, Wiley-VCH.
2. Edelstein, A.S., & Cammarata, R.C. (2001). Nanomaterials: Synthesis, properties, and applications. CRC Press, 1st edition, 2001.
3. Rao, C.N.R., & Müller, A. (2003). Nanomaterials chemistry: A review of the scientific and technological aspects. World Scientific 1st Edition.
4. Vollath, D. (2008). Nanomaterials: Synthesis, characterization, and applications, 1st Edition, Wiley-VCH.

Reference Books:

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

Weblinks:

1. https://onlinecourses.nptel.ac.in/noc21_mm38/preview
2. 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.

Textbooks:

1. "Radiochemistry and Nuclear Chemistry" by Gregory Choppin, Jan-Olov Liljenzin, Jan Rydberg, 3rd Edition, Elsevier, 2013.
2. "Nuclear and Radiochemistry: Fundamentals and Applications" by Karl Heinrich Lieser, 1st edition, Wiley- VCH, 2001.
3. "Introduction to Nuclear Chemistry" by Harold C. Beard, 1st Edition, Prentice Hall, 1969.

Reference Books:

1. "Fundamentals of Radiation Chemistry" by A. Mozumder, Y. Hatano. 1st 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, 1st edition, 1997.
2. C.M.A. Brett and A.M.O. Brett, Electroanalysis, Oxford Chemistry Primers, Oxford Science Publications, 1st Edition, 1988.
3. J. Janata, 1989, 1st Edition, Principles of Chemical Sensors, Plenum Press, New York.

Reference Books:

1. Chemical Sensors, Chapman and Hall, New York T. E. Edmonds (ed.), 1st Editon, 1988.

Weblinks:

1. **https://onlinecourses.nptel.ac.in/noc23_ee95/preview**
2. **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_2, NBS, peracids, Prevost dihydroxylation, Woodward's modified dihydroxylation, chromium (VI) oxidants, $KMnO_4$, OsO_4, MnO_2, Ag_2CO_3, $Pb(OAc)_4$, and HIO_4. 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 $LiAlH_4$ and its derivatives, $NaBH_4$ 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. Part A: Structure and Mechanisms, Francis A. Carey and Richard J. Sundberg University of Virginia, Charlottesville, Virginia, 5th Editon, Springer, 2007
2. Part B: Reactions and Synthesis, Francis A. Carey and Richard J. Sundberg, University of Virginia, Charlottesville, Virginia, 5th Editon, Springer, 2007.
3. "Organic Chemistry" by R. T. Morrison and R. N. Boyd ,Prentice Hall, 6th Editon, 1992.

Reference Books:

1. "Modern Organic Synthesis: An Introduction" by George S. Zweifel and Michael He Nantz, University of California, Wiley, 1st Edition, , 2007.
2. W. Carruthers and Iain Coldham, "Modern Methods of Organic Synthesis," Cambridge University Press, 4th 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; homologation; bioisostere; chain branching; Electronic effects; Lipophilicity; Structure-Activity Relationships; Quantiative-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; Oxford University Press, 2nd Edition, 2001.
2. The Organic Chemistry of Drug Design and Drug Action, Richard B. Silverman, 2nd Edition, Elsevier, 2004.

Reference Books:

1. Lehninger's Principles of Biochemistry, Cox and Nelson, WH Freeman & Co, 5th Edition , 2008.

2. Foye's Principles of Medicinal Chemistry, Foye, W. O., Lemke, T. L., & Williams, D. A, Wolters Kluwer Health, 8th Edition, 2019.

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Weblinks:

1. **https://onlinecourses.nptel.ac.in/noc25_cy22/preview**
2. **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" by Paul T. Anastas and John C. Warner, 1st Edition, Oxford University Press, 1998.
2. "Introduction to Green Chemistry" by Albert S. Matlack, 1st Edition, Marcel Dekker, 2001.
3. "Sustainable Industrial Chemistry: Tools and Principles" by Fabrizio Cavani, Gabriele Centi, and Siglinda Perathoner, 1st Editon, Wiley-VCH, 2014.

Reference Books:

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

Weblinks:

1. **https://onlinecourses.nptel.ac.in/noc21_mg85/previ**
2. **https://onlinecourses.nptel.ac.in/noc23_ge17/preview**

Environmental Quality Monitoring & Analysis

Course Code: 246CH010

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, Koc, Kow 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, , Wiley-Inter science, 2nd Edition , 2009.
2. Environmental Engineering – Peavy, Rowe and Tchobanoglous, McGraw- Hill, 1st Edition,1985.

Reference Books:

1. Atmospheric Chemistry and Physics – Seinfeld and Pandis, Wiley- Inter Science, 2nd Editon,2006.

Weblinks:

1. **https://onlinecourses.nptel.ac.in/noc21_ch13/preview**
2. **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" by S.K. Garg, Khanna Publishers, 1st Edition, 2004.
2. "Water and Wastewater Technology" by Mark J. Hammer and Mark J. Hammer Jr., , Prentice Hall ,6th Edition, 2008.

Reference Books:

1. "Industrial Wastewater Treatment" by A.D. Patwardhan, Narosa Publishing House, 1st Edition, 2001.

Weblinks:

1. **https://onlinecourses.nptel.ac.in/noc25_ce33/preview.**
2. **https://onlinecourses.nptel.ac.in/noc24_ce105/preview**