

**B.Sc. (Analytical Chemistry)  
(Chemistry Component)**

**Semester-wise Distribution of DSC, DSE and GE Courses**

Semester	Course type	NAME OF THE COURSE	Credits
<b>VII</b>	<b>DSC-19</b>	<b>ADVANCED INSTRUMENTAL METHODS 1</b>	<b>T=3; P=1</b>
	<b>DSE-6</b>	<b>MATERIALS SCIENCE</b>	<b>T=2; P=2</b>
	<b>DSE-7</b>	<b>COMPUTATIONAL METHODS AND MOLECULAR MODELLING</b>	<b>T=2; P=2</b>
	<b>DSE-8*</b>	<b>FUNDAMENTALS OF MEDICINAL CHEMISTRY</b>	<b>T=2; P=2</b>
	<b>GE</b>	<b>GREEN ENERGY SOLUTIONS</b>	<b>T=2; P=2</b>
<b>VIII</b>	<b>DSC-20</b>	<b>ADVANCED INSTRUMENTAL METHODS II</b>	<b>T=3; P=1</b>
	<b>DSE-9</b>	<b>CHEMINFORMATICS</b>	<b>T=2; P=2</b>
	<b>DSE-10</b>	<b>CHEMICAL PATENT ANALYTICS &amp; IP STRATEGY</b>	<b>T=2; P=2</b>
	<b>DSE-11*</b>	<b>INTRODUCTORY INTERFACIAL ELECTROCHEMISTRY</b>	<b>T=2; P=2</b>
	<b>GE</b>	<b>INDUSTRIAL POLLUTION-IMPACTS&amp; REMIDIES</b>	<b>T=2; P=2</b>

**NOTE:\*** For syllabus content of Discipline Specific Elective-8 (DSE-8) “Fundamentals of Medicinal Chemistry” and Discipline Specific Elective-11 (DSE-11) “Introductory Interfacial Electrochemistry” refer to DSE syllabus of B.Sc. (Physical Sciences)

## SEMESTER VII

### DISCIPLINE SPECIFIC CORE COURSE-19

#### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
ADVANCED INSTRUMENTAL METHODS 1	4	3	0	1	12 <sup>th</sup> Class: Physics, Chemistry, Mathematics	-

#### Course Objectives:

- To introduce the students to advanced techniques in molecular structure elucidation using instrumental methods.
- To provide theoretical and practical knowledge of Mass Spectrometry and Nuclear Magnetic Resonance Spectroscopy.
- To develop skills for interpreting spectral data and deducing the structure of unknown compounds using a combination of techniques.

#### Learning Outcomes:

By the end of this course, students will be able to learn:

- Interpret and analyze mass spectra to identify molecular weights and fragment patterns.
- Understand and apply 1D and 2D NMR techniques in structural elucidation.
- Integrate data from UV-Vis, IR, NMR, and MS to deduce complex molecular structures.
- Perform hands-on experiments using spectroscopy instrumentation and software tools for spectral interpretation.

### SYLLABUS OF DSC- 19

#### THEORY COMPONENT

##### UNIT 1: Mass Spectrometry (15 Hours)

**Basic principles:** Instrumentation: Sample Inlet system,

**Ionization techniques;** (EI, CI, ESI, MALDI, API, FAB), Mass analysers: Quadrupole, Time-of-Flight (TOF), Magnetic Sector, Radius of ion, Orbitrap, FT-ICR. Positive fragment ions peak, metastable peak, isotopic mass peaks, Recognition of  $M^+$  Peak, singly, doubly and

multiply charged ions. General fragmentation rules and fragmentation of different classes of compounds, factors governing general fragmentation processes, Mc Lafferty Rearrangement and Ortho effect, Nitrogen rule, Rule 13.

**Applications:** High-resolution mass spectrometry (HRMS), isotope patterns, exact mass, tandem MS (MS/MS). Use known compounds for spectrum-based analysis: **Acetophenone** (Analyze fragmentation and base peak formation), **n-Butylamine** (Use nitrogen rule and  $\alpha$ -cleavage pathways), **Toluene** (Observe loss of  $\text{CH}_3$  and formation of tropylium ion ( $m/z$  91)), **Methionine (amino acid)**: Apply ESI and analyze isotope peaks for sulfur.

## **UNIT 2: Advanced NMR Spectroscopy (15 Hours)**

**$^{13}\text{C}$  NMR Spectroscopy:** Natural abundance, resolution and multiplicity of  $^{13}\text{C}$  NMR,  $^1\text{H}$  decoupling, noise decoupling, broad band decoupling, Deuterium, fluorine coupling; NOE signal enhancement, off-resonance, DEPT (Distortionless Enhancement by Polarization Transfer): DEPT-45, DEPT-90, DEPT-135 (Identify  $\text{CH}_3$ ,  $\text{CH}_2$ ,  $\text{CH}$ , and quaternary carbons in ethylbenzene).

**Two-Dimensional Nuclear Magnetic Resonance Spectroscopy (2D NMR):** Basic introduction of 2D NMR, The spin-echo experiment, multi-pulse NMR, Homonuclear correlation experiments (COSY), Heteronuclear correlation (HETCOR, HMQC, HSQC), NOE experiments (NOESY, HOESY, ROESY), and INADEQUATE, Exchange Spectroscopy (ESXY)

**Variable Temperature and Dynamic NMR:** Study of conformational changes and fluxional behavior, Coalescence temperature and line shape analysis, Arrhenius/Eyring plots for rate constant determination, **VT NMR** of N,N-dimethylformamide (DMF): Observe restricted rotation of  $\text{N}-\text{CH}_3$  groups at low temperatures, **Dynamic NMR** of cyclohexane: Detect chair inversion and estimate activation barrier.

**Solid-State NMR (Basics Only),** Magic Angle Spinning (MAS), Cross-Polarization (CP-MAS).

## **UNIT 3: Structure Elucidation(7 Hours)**

Structure elucidation of complex organic compounds based on  $^1\text{H}$ -NMR,  $^{13}\text{C}$ -NMR, 2D NMR, IR, UV, and MS spectral data: Functional group identification, fragment identification, connectivity, symmetry, diastereotopicity, shielding/deshielding effects, spin-spin coupling, exchangeable protons. Contour plot reading and identification of interactions.

## **UNIT 4:Quantitative NMR (8 Hours)**

Quantitative NMR (qNMR): Principles of quantitation using NMR, proportionality of signal intensity and number of nuclei, factors affecting accuracy: relaxation time ( $T_1$ ), pulse angle, acquisition time. Applications of qNMR: Purity determination, quantification of mixture, stability study, degradation/reaction/process monitoring, intermediate identification, etc,

Use of spectral databases (NIST, SDBS, ChemSpider), Introduction to software: MestReNova, Delta JEOL, ACD/NMR, Bruker TopSpin, ChemDraw for spectra simulation.

## PRACTICAL COMPONENT (30 Hours)

1. Identify the possible fragment ions for the following classes of compounds (Provide the mass spectra and discuss the fragmentation processes)
  - a) Alkyl-substituted benzenes
  - b) Phenols
  - c) Aldehydes and ketones
  - d) Esters
  - e) Amines
  - f) Nitro compounds
  - g) Alkyl halides
2. Process the given FID files of NMR spectra using any NMR processing software, and identify the compound (Provide the molecular formula)
3. Record the NMR spectra of simple organic compounds, simulate the NMR spectra of same compounds using ACD/NMR, ChemDraw, MestReNova or any other software, and compare the results.
4. Elucidate the structure of organic compounds using UV-Vis, MS, IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR (Provide the spectral data).
5. Interpret 2D NMR spectra of organic molecules (provide the spectra).
6. Estimate the percentage of purity or percentage of isomers using the given  $^1\text{H}$  NMR spectrum.
7. Analyze  $^{13}\text{C}$  CP-MAS data of polymers or crystalline drugs (Identify carbon environments and discuss applications)

## RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

### Theory:

1. Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R., Introduction to Spectroscopy (5th Edition) – Cengage Learning
2. Silverstein, R. M., Webster, F. X., & Kiemle, D. J., Spectrometric Identification of Organic Compounds (7th Edition) – Wiley
3. Williams, D. H., & Fleming, I., Spectroscopic Methods in Organic Chemistry (6th Edition) – McGraw Hill
4. Lambert, J. B., Shurvell, H. F., Lightner, D. A., & Cooks, R. G., Organic Structural Spectroscopy – Pearson
5. Claridge, T. D. W., High-Resolution NMR Techniques in Organic Chemistry – Elsevier

### Practicals:

1. Pavia, D. L., Lampman, G. M., Kriz, G. S., Introduction to Organic Laboratory Techniques – Cengage
2. Instrumental manuals and user guides (Bruker, JEOL, Thermo, Agilent etc.)
3. Online Platforms:
  - Spectral Database for Organic Compounds (SDBS)
  - ChemSpider
  - NIST

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

## DISCIPLINE SPECIFIC ELECTIVE6

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>MATERIAL SCIENCE</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>NIL</b>

#### Course Objectives:

- Understand the fundamental chemistry behind smart and responsive materials.
- Analyze how external stimuli affect chemical and physical behavior.
- Apply smart material concepts to emerging technologies and real-world applications.
- To provide a scientific understanding of composite materials, including their classification, synthesis, chemical behavior, and analytical characterization.
- To develop hands-on skills in preparing and analyzing composite materials using standard instrumental techniques.

#### Learning Outcomes

By the end of this course, students will be able to:

1. Define and classify various smart materials based on their responsiveness.
2. Describe the molecular-level mechanisms that govern smart behavior.
3. Analyze real-life applications of smart materials in biomedical, industrial, and environmental domains.
4. Classify different types of composite materials and explain matrix-reinforcement chemistry.
5. Prepare basic polymer composites using hand lay-up methods.
6. Critically assess real-life applications of composite materials in different industries.

### THEORY COMPONENT

#### UNIT 1: Smart Materials

(9 hours)

**Introduction to Smart Materials** - Definitions, history, and importance; Types and classifications; General applications

**Molecular Basis of Responsiveness** - Stimuli-responsive mechanisms; Molecular interactions and chemical triggers; reversible behaviour

**Shape Memory Materials** - Alloys (e.g., Nitinol) and shape memory polymers; Mechanistic explanation; Biomedical and structural applications

**Thermo- and pH-Responsive Polymers** - Polymer behaviour with temperature and pH; LCST and UCST phenomena.

**Photo-responsive Materials** - Cis-trans isomerization (azobenzene, spiropyran); Photochromism and molecular switches; Smart windows, data storage

**Electrochromic and Piezoelectric Materials** - Redox-induced optical changes; Electric field-induced mechanical response; Applications in flexible electronics and wearables

**Self-Healing Materials** - Micro-encapsulation and polymer chemistry; Intrinsic vs extrinsic healing; Aerospace, electronics, and coatings.

**Smart Coatings and Textiles** - Responsive surfaces; Moisture, temperature, and pollutant-sensitive textiles; Industrial and military applications

**Emerging Trends and Future Prospects** - 4D printing, adaptive materials, AI-integrated materials; Challenges: cost, scalability, and environmental impact; Career and research opportunities

## **UNIT 2: Composite Materials**

**(6 hours)**

**Fundamentals of Composites:** Definition and importance of composite materials, Classification: PMC (Polymer Matrix Composites), MMC (Metal Matrix Composites), CMC (Ceramic Matrix Composites), Basic matrix-filler concept, Real-world examples (building materials, bicycles, sports goods)

**Reinforcement Interaction & Matrix Chemistry:** Molecular bonding between filler and matrix (simplified), Interface chemistry (basic idea of bonding), Types of polymers: Thermosets vs. Thermoplastics, Functional groups in epoxy and polyester (only basic structural features), Role of initiators and crosslinkers

**Curing & Composite Preparation Techniques:** Curing process and epoxy hardening (with visuals), Coupling agents like silanes, Preparation methods (conceptual only): Hand lay-up, Extrusion, Compression molding, Spray lay-up, Vacuum bagging & autoclave (demonstration-based understanding)

## **UNIT 3: Biomaterials**

**(9 hours)**

**Introduction to Biomaterials:** Definition and scope of biomaterials, historical development and milestones, classification: metals, ceramics, polymers, composites, and natural biomaterials. Key properties: Biocompatibility, biodegradability, mechanical strength, and surface characteristics.

### **Biomaterials in Medical Applications**

**Orthopedic Biomaterials:** Metals (titanium, stainless steel, Co-Cr alloys), bioactive ceramics (hydroxyapatite, bioglass), polymer composites for joint replacements and bone grafts.

**Cardiovascular Biomaterials:** Stents (bare-metal, drug-eluting, bioresorbable), heart valves (mechanical vs. tissue-based), vascular grafts and artificial blood vessels.

**Dental Biomaterials:** Dental implants (titanium, zirconia), restorative materials (composites, ceramics, amalgams), biodegradable scaffolds for periodontal regeneration.

**Biomimetic and Bio-inspired Materials** - Learning from nature (e.g., lotus effect, gecko adhesion); Supramolecular chemistry; Applications in tissue scaffolding and robotics, natural vs. synthetic scaffolds (collagen, PLGA, PCL), material used in skin, cartilage, and bone regeneration.

## **UNIT 4: Characterization Techniques:**

**(6 hours)**

**Characterization Techniques:** FTIR, UV-Vis, CHNS, TGA/DTG, DSC, SEM/EDX

**Stability, Surface & Real-World Applications:** Degradation under acidic and basic media, Leaching and environmental testing, Surface morphology: Cracks, bonding, fiber-pull, Application case studies:

- Fly-ash/glass fiber composites in buildings
- Carbon fiber in cars/planes
- Bio-composites in packaging/medical uses
- Corrosion-resistant composites in coastal infrastructure

## **PRACTICAL COMPONENT (60Hours)**

1. Thermo-responsive Polymer Gel: Synthesize poly(N-isopropylacrylamide) and demonstrate phase transition at LCST.
2. Shape Memory Wire Demonstration: Heat and recover shape of Nitinol wire.
3. Photochromic Dye Experiment: Use spiropyran or azobenzene-based materials and expose to UV light.
4. pH-Sensitive Color Change: Use anthocyanin extract or pH indicators in polymer films.
5. Electrochromic Device Prototype: Build a simple setup using a viologen-based electrochromic material.
6. Bioinspired Surface: Prepare lotus-leaf-mimicking superhydrophobic surface using candle soot or nanoparticle coatings.
7. Preparation of a Glass-Fiber Reinforced Epoxy Composite: To prepare and understand the hand lay-up method and curing.
8. FTIR Analysis of Uncured vs Cured Epoxy Composite: To study functional group changes during curing, IR peaks (C=O, OH, epoxy ring), crosslinking evidence.
9. Thermal Stability by TGA: To determine the decomposition temperature of the polymer composite, Mass loss curve interpretation.
10. Surface Morphology by SEM (demonstration/image analysis): To observe surface topology, fiber pull-out, cracks, SEM image interpretation.
11. pH and Ion Leaching Test of Composites: To assess chemical stability under acidic/basic media, Leachate analysis using pH/conductivity meter or titration.

## **RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES**

### **Theory**

1. "Smart Materials and Structures" by M.V. Gandhi and B.S. Thompson
2. "Smart Materials in Structural Health Monitoring, Control and Biomechanics" by Chee K. Tan
3. "Stimuli-Responsive Materials: From Molecules to Nature Mimicking Materials Design" by Qiang Zhao and Tao Xie
4. Selected research articles and review papers (to be provided per topic)
5. K.K. Chawla, *Composite Materials: Science and Engineering*
6. D.D.L. Chung, *Functional Materials: Composites and Hybrid Systems*
7. R.F. Speyer, *Thermal Analysis of Materials*
8. Research Articles from *Polymer Composites*, *Composites Part A*, *Journal of Applied Polymer Science*
9. ASTM/ISO standards for composite testing (optional for PG)

### **Practicals**

1. Smith, B. C. *Infrared Spectral Interpretation: A Systematic Approach*, CRC Press.
2. Silverstein, R. M., et al. *Spectrometric Identification of Organic Compounds*, Wiley

3. Speyer, R. F. *Thermal Analysis of Materials*, Marcel Dekker, 1994.
4. Hatakeyama, H. & Hatakeyama, T. *Thermal Analysis: Fundamentals and Applications to Polymer Science*, Springer.
5. Goldstein, J. I., et al. *Scanning Electron Microscopy and X-ray Microanalysis*, Springer.
6. Skoog, D. A., Holler, F. J., & Crouch, S. R. *Principles of Instrumental Analysis*, Cengage Learning.
7. Sparks, D. L. *Environmental Soil Chemistry*, Academic Press. (For leaching relevance).
8. Callister, W. D., & Rethwisch, D. G. *Materials Science and Engineering Laboratory Manual*, Wiley.

**Suggested readings:**

1. Ratner, B. D., Hoffman, A. S., Schoen, F. J., & Lemons, J. E. *Biomaterials Science: An Introduction to Materials in Medicine* (3rd Edition) - Academic Press
2. Park, J., & Lakes, R. S. *Biomaterials: An Introduction* (3rd Edition) - Springer
3. Williams, D. F. *The Biomaterials: Silver Jubilee Compendium* - Elsevier
4. Ong, K. L. *Orthopedic Biomaterials in Research and Practice* - Springer
5. How, T. V., & Black, R. A. *Biomaterials and Devices for the Circulatory System* – Woodhead
6. Lanza, R., Langer, R., & Vacanti, J. *Principles of Tissue Engineering* (5th Edition) - Academic Press
7. Al-Shibouri, A. M., & Nimesh, S. *Engineering Drug Delivery Systems* - Elsevier

**Online Resources:**

1. National Institute of Biomedical Imaging and Bioengineering: <https://www.nibib.nih.gov>
2. Materials Today Biomaterials <https://www.materialstoday.com/biomaterials>

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## DISCIPLINE SPECIFIC ELECTIVE 7

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>COMPUTATIONAL METHODS AND MOLECULAR MODELLING</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>-</b>

#### Course Objectives:

- To make students learn the theoretical background of computational techniques in molecular modelling.
- To give the different flavours of computational chemistry by the end of this course.
- To provide hands-on experience in molecular modelling on various software

#### Learning Outcomes:

Students will be able to:

- Explain the theoretical background of computational techniques and selective application to various molecular systems
- Compare computational and experimental results and explain deviations.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through the use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.
- Perform analysis of molecular properties using various software

#### **UNIT 1: Introduction (6 hours)**

Introduction to computational chemistry: Overview of Classical and Quantum Mechanical Methods (Ab initio, DFT, Semi-empirical, Molecular Mechanics, Molecular Dynamics, and Monte Carlo)

#### **UNIT 2: Potential Energy Surfaces (6 hours)**

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global

minima, Geometry optimization and energy minimization, the concept of transition state with examples, Hessian matrix

### **UNIT 3: Molecular Mechanics & Molecular Dynamics (6 hours)**

#### ***Molecular Mechanics:***

Force Fields (A brief explanation of all the terms of a basic force field), parametrising a force field, the basic idea of MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.

#### ***Molecular Dynamics:***

The concept of the periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), steps in a typical MD simulation.

### **UNIT 4: Huckel Molecular Orbital Theory (12 hours)**

Huckel MO with examples: ethene and propenyl systems, Properties calculated – energy, charges, bond order, electronic energies, resonance energies.

#### ***Ab-Initio Methods***

Antisymmetry principle, Slater determinants, SCF method, Hartree-Fock method.

Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets

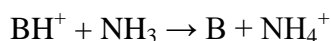
### **Practicals**

**(60 hours)**

*Any 8 -10 Problems*

1. Write the Z-Matrix of a given set of molecules.
2. Carry out geometry optimisation on H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se molecules compare the optimized bond angles and dipole moments from the results obtained. Obtain the ESP-mapped density surfaces and interpret the results obtained with reference to bonding in these molecules.
3. Calculate the energy of the following chemical species and arrange them in order of increasing stability:  
  
1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.
4. Carry out geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules:  
  
1-pentanol, 2-pentanol, 3-pentanol, 2-methyl butan-1-ol, 3-methyl butan-1-ol, 2-methyl butan-2-ol, 2-methyl butan-3-ol and 2,2-dimethyl propanol.
5. Based on the implicit electronic structure calculations, determine the heat of hydrogenation of Propylene.
6. Based on the calculations of enthalpies of the participating chemical species on the optimized geometry of the molecules, calculate the reaction enthalpy at 298K of (a) Steam reforming of methane (b) Haber-Bosch Process
7. Carry out geometry optimisation & Energy calculations on Benzene, Naphthalene, and Anthracene. Obtain Frontier Molecular Orbitals, visualise the Molecular Orbitals of these species, and interpret the results for bonding in these molecules.

8. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:



Where B =  $\text{CH}_3\text{NH}_2$ ,  $(\text{CH}_3)_2\text{NH}$ ,  $(\text{CH}_3)_3\text{N}$

9. Based on the results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis and trans 2-butene.
10. Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.
11. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
12. Calculate the electronic UV/Visible absorption spectrum of Benzene.
13. Calculate the electronic absorption spectra of formaldehyde.
14. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.

### RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

#### Theory:

- Lewars, E. (2003), Computational Chemistry, Kluwer academic Publisher.
- Cramer, C.J. (2004), Essentials of Computational Chemistry, John Wiley & Sons.
- Hinchcliffe, A. (1996), Modelling Molecular Structures, John Wiley & Sons.
- Leach, A.R. (2001), Molecular Modelling, Prentice-Hall.
- House, J.E. (2004), Fundamentals of Quantum Chemistry, 2nd Edition, Elsevier.
- McQuarrie, D.A. (2016), Quantum Chemistry, Viva Books.
- Levine, I. N.; Physical Chemistry, 5th Edition, McGraw –Hill.

#### Practicals

- [https://www.afs.enea.it/software/orca/orca\\_manual\\_4\\_2\\_1.pdf](https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf)
- <https://dasher.wustl.edu/chem430/software/avogadro/learning-avogadro.pdf>
- <http://www.arguslab.com/arguslab.com/ArgusLab.html>
- <https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf>
- <https://gaussian.com/techsupport/>
- <https://gaussian.com/man/>
- <https://gaussian.com/wp-content/uploads/dl/gv6.pdf>
- <https://dasher.wustl.edu/chem478/software/spartan-manual.pdf>
- <http://www.mdtutorials.com/gmx/>
- <https://vina.scripps.edu/manual/>

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## DISCIPLINE SPECIFIC ELECTIVE 8

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>INTRODUCTORY INTERFACIAL ELECTROCHEMISTRY</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>-</b>

**\*\*For syllabus content of Discipline Specific Elective-8: (DSE-8) “Introductory Interfacial Electrochemistry” refer to the syllabus content of DSE-18 PS of B Sc. Physical Sciences Programme.**

## GENERIC ELECTIVE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>GREEN ENERGY SOLUTIONS</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>-</b>

### Course Objectives:

- Introduce core concepts in renewable and non-renewable energy
- Explain the science behind clean energy technologies
- Provide insight into India's current green energy initiatives
- Familiarize students with practical tools, energy efficiency, and storage systems
- Create awareness about policy, innovation, and future career opportunities in energy

### Learning Outcomes:

Students will be able to:

- Identify major renewable energy systems and their underlying science
- Estimate solar potential using simulation tools
- Understand India's energy policies, electric mobility plans, and startup innovations
- Apply basic energy audit and comparative assessment techniques
- Participate in group-based exploration and communication of green energy ideas

### THEORY:

#### Unit 1: Energy and the Environment (6 Hours)

- Forms of energy; renewable vs non-renewable
- Fossil fuels: sources, use, and environmental impact
- India's energy consumption profile
- Environmental consequences: air pollution, greenhouse gases, climate change
- Traditional Indian energy practices and their sustainability insights

#### Unit 2: Solar and Hydrogen Energy (8 Hours)

- Basics of solar energy: photovoltaic effect, solar thermal systems
- Types of solar panels: monocrystalline, polycrystalline (basic comparison)
- Components and layout of a small solar system, perovskite solar cells
- Hydrogen as a fuel: green hydrogen electrolysis, properties, use cases, safety
- Fuel cells: basic working principle and relevance in transportation
- India's solar programs and National Green Hydrogen Mission

#### Unit 3: Biofuels, Batteries, and Energy Storage (8 Hours)

- Types of biofuels: ethanol, biodiesel, biogas – preparation, chemistry, benefits
- Battery technologies: lead-acid, lithium-ion – structure, function, and applications
- Importance of grid-level storage and stability
- Energy storage methods: pumped hydro, BESS, and battery-integrated solar setups
- Electric Vehicles as mobile storage; Battery swapping and EV charging ecosystem
- India's FAME scheme and emerging EV landscape

#### Unit 4: Energy Efficiency, Policy, and Innovation (8 Hours)

- Energy-efficient appliances, conservation practices, behavioral changes
- Carbon footprint: meaning, impact, and mitigation
- Life Cycle Analysis (LCA): basic concept and real-life examples
- Key Indian government programs: UJALA, PM-KUSUM, FAME, Green Hydrogen Mission
- Carbon markets and energy pricing (simplified overview)
- Indian startups and innovations in green energy: ReNew, Ather, Log9, Ola Electric

## PRACTICALS

Any 8 Activities + 1 Group Project optional

1. Compare visible smoke and residue from different fuel types (wood, kerosene, LPG – demo)
2. Create and test a fruit or salt-water battery
3. Prepare simple biodiesel from vegetable oil (under supervision)
3. Estimate rooftop solar output using MNRE Solar Calculator or RETScreen (guided worksheet)
4. Conduct a home/college room energy audit (appliances, lighting, fan usage)
5. Compare energy-efficient vs conventional appliances (e.g., LED vs CFL)
6. Poster/model or infographic on one major Indian energy initiative or clean-tech startup
7. Survey-based project: public awareness of solar/EVs in your locality
8. Group project + viva presentation on a selected green energy theme

## Suggested Readings

- *Energy Resources and Utilization* – K. S. Ramaswamy (Narosa Publishing)
- *Environmental Chemistry and Pollution Control* – S. S. Dara (S. Chand)
- *Renewable Energy and Environment* – Mukesh Khare & R. K. Anand (Narendra Publishing)
- Selected articles from *Down to Earth* – Centre for Science and Environment (CSE)
- Government PDFs and online documents from MNRE, FAME India, and UJALA portals

**Note:** Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

## SEMESTER VIII

### DISCIPLINE SPECIFIC CORE COURSE-20

#### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
ADVANCED INSTRUMENTAL METHODS II	4	3	0	1	12 <sup>th</sup> Class: Physics, Chemistry, Mathematics	-

#### Course Objectives:

- To provide fundamental and applied knowledge of thermal and surface analytical techniques.
- To enable students to understand the principles and instrumentation of thermal analysis and nanostructure characterization.
- To interpret data from TGA, DTA, DSC, SEM, and TEM for material identification and behavior analysis.

#### Learning Outcomes:

By the end of the course, students will be able to:

- Understand the principles and instrumentation of thermal analysis (TGA, DTA, DSC).
- Apply thermal techniques to analyze thermal stability, decomposition, and transitions of materials.
- Understand the working, imaging principles, and resolution differences between SEM and TEM.
- Analyze nanoscale morphology, particle size, and surface features using SEM and TEM data.
- Conduct basic data interpretation and material characterization using experimental tools and simulation software.

#### THEORY:

##### UNIT 1: Introduction to Thermal Analysis (10 Hours)

Overview of thermal methods: Thermogravimetric Analysis (TGA), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Classification: Dynamic and Isothermal techniques, Comparative overview: TGA, DTA, DSC, TMA (Thermomechanical Analysis), and DMA (Dynamic Mechanical Analysis), Importance of thermal analysis in materials science, pharmaceuticals, polymers, and food technology, Types of Samples and

Sample Handling: Sample forms: powders, solids, films, liquids, Factors affecting thermal behavior: mass, particle size, packing, thermal conductivity, Sample pans: crucible materials (alumina, platinum, aluminum), Calibration and Standardization: Instrument calibration using reference materials (e.g., indium, tin, lead for DSC), Baseline correction, temperature calibration, and sensitivity testing, Importance of reproducibility and blank run procedures, Factors Influencing Thermal Curves: Instrumental parameters: heating rate, gas flow rate, crucible type, Environmental effects: humidity, atmospheric pressure, Interaction with container walls or decomposition gases

## **UNIT 2: Thermogravimetric Analysis (TGA) (10 Hours)**

**Thermogravimetric Analysis (TGA)** – Basic Concepts, Principle and instrumentation of TGA, Thermogram interpretation: weight loss, multi-step decomposition, Analysis of  $\text{CaCO}_3$  decomposition, Thermal stability of polymers and metal complexes, Significance of inert ( $\text{N}_2$ ) and oxidative ( $\text{O}_2$ , air) atmospheres, TGA coupled with **mass spectrometry (TGA-MS)** for evolved gas analysis, TGA-FTIR for gas-phase identification of decomposition product.

## **UNIT 3: DSC and DTA (10 Hours)**

**Differential Scanning Calorimetry (DSC)** – Basic Concepts, Heat flow vs. temperature curves, Principle and comparison of DTA vs. DSC, Endothermic and exothermic transitions, Determination of melting point, glass transition temperature ( $T_g$ ), crystallinity, Heat capacity and enthalpy measurements, Phase transition of polyethylene, Crystallinity changes in semicrystalline polymers, Enthalpy of fusion for organic solids, Applications in food additives, drug formulation, and polymer quality control. **Differential Thermal Analysis (DTA)** – Basic Concepts, Principle of differential temperature measurement between sample and reference, Typical DTA curves and interpretation: endothermic/exothermic events, Instrument setup and thermocouple configurations, **Classification of Thermal Techniques**, Dynamic vs. Isothermal methods, Static vs. programmed heating, Importance of heating/cooling rates and sample holder selection.

## **UNIT 4: Introduction to Nanomaterials and Electron Microscopy (15 Hours)**

Basics of nanomaterials: size, surface effects, properties, Introduction to imaging: resolution, contrast, magnification, Electron-material interaction and signal generation, **Scanning Electron Microscopy (SEM)**: Working principle and instrumentation of SEM, Secondary electron and backscattered electron imaging, Sample preparation and gold coating, Surface topology, morphology, particle shape analysis, SEM of nanoparticles, corrosion pits, biological materials, **Transmission Electron Microscopy (TEM)**: Principle and instrumentation of TEM, Electron diffraction, contrast mechanisms, High-resolution TEM (HRTEM), Sample thinning techniques, TEM images of metal nanoparticles, nanorods, and carbon nanotubes, Crystallite size and lattice fringes.

## **PRACTICAL COMPONENTS (30 Hours)**

1. Thermogravimetric Analysis (TGA) of hydrated salts or polymers. Record weight loss and analyze decomposition steps.
2. DSC analysis of pure organic compounds and polymers. Measure melting point, glass transition, and enthalpy.
3. DTA of a multicomponent inorganic salt. Identify endothermic and exothermic transitions.
4. Interpretation of recorded TGA/DSC thermograms from literature or instruments.



5. SEM image analysis using provided micrographs. Measure particle size, surface texture, and morphology.
6. TEM micrograph interpretation. Determine lattice fringes, particle shape, and crystallite boundaries.
7. Visit/demo of SEM/TEM facility (if available). Instrument components, vacuum system, sample mounting.
8. Software simulation of electron beam interactions. Use open-source or institutional software for understanding signal generation.

## ESSENTIAL/RECOMMENDED TEXTBOOKS

### Theory:

1. **Skoog, Holler, and Crouch**, *Principles of Instrumental Analysis* (7th Ed.) – Cengage
2. **Willard, Merritt, Dean, and Settle**, *Instrumental Methods of Analysis* – CBS Publishers
3. **Tiwari, Ashutosh**, *Nanomaterials: A Guide to Fabrication and Applications* – Wiley
4. **Ertl, G., Knözinger, H., & Weitkamp, J.**, *Handbook of Heterogeneous Catalysis (vol. 1: Characterization Techniques)* – Wiley-VCH
5. **Brown, M.E.**, *Introduction to Thermal Analysis: Techniques and Applications* – Springer
6. **N.K. Kaushik and Shulka**, *Thermal Analysis Techniques and Applications*, IK International.

### Practicals and Data Interpretation:

1. Practical Manual of Instrumental Techniques for Chemistry Students – University-level lab manuals
2. Lab Guide for Materials Characterization – Any departmental handout or material characterization facility guide
3. SEM/TEM Micrograph Interpretation Manual – Available from JEOL/FEI training resources
4. Online Spectral/Imaging Databases – NIMS, SpringerMaterials, NIST, etc.

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## DISCIPLINE SPECIFIC ELECTIVE9

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
CHEMINFORMATICS	4	2	0	2	12 <sup>th</sup> Class: Physics, Chemistry, Mathematics	-

#### Course Objectives:

- The aim of the course is to introduce the students to computational drug design through structure-activity relationship, QSAR and combinatorial chemistry. The students will learn about the target analysis, virtual screening for lead discovery, structure based and ligand-based design method and the use of computational techniques, library preparation and data handling.

#### Learning Outcomes:

By the end of the course, the students will be able to:

- Have a comprehensive understanding of drug discovery process and techniques including structure-activity relationship, quantitative structure activity relationship and the use of cheminformatics in this, including molecular modelling and docking studies.
- Appreciate role of modern computation techniques in the drug discovery process and perform their own modelling studies.

#### THEORY:

##### UNIT 1: (4hours)

Introduction to Cheminformatics: History and evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular modelling and structure elucidation.

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

##### UNIT 2: (12hours)

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity.

**UNIT3: (6 hours)**

Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design

**UNIT4: (8 hours)**

Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Cheminformatics in Drug Design.

**Practical: (60 hours)**

1. Overview of Rational Drug Design, Ligands and Targets
2. In silico representation of chemical information
  - i. CIF IUCr Crystallographic Information Framework
  - ii. CML Chemical Markup Language
  - iii. SMILES -- Simplified Molecular Input Line Entry Specification
  - iv. InChi -- IUPAC International Chemical Identifier
3. Chemical Databases and Data Mining
  - i. Cambridge Structural Database CCDC CSD
  - ii. Crystallographic Open Database COD
  - iii. Protein Data Bank PDB Ligand Explorer
  - iv. Chempider
4. Molecular Drawing and Interactive Visualization
  - i. ChemDraw
  - ii. MarvinSketch
  - iii. ORTEP
  - iv. Chimera, RasMol, PyMol
5. Computer-Aided Drug Design Tools
  - i. Molecular Modeling Tools
  - ii. Structural Homology Modeling Tools
  - iii. Docking Tools and Screening Tools
6. Building a Ligand
  - i. Building ab initio
  - ii. Building from similar ligands
  - iii. Building with a known macromolecular target
  - iv. Building without a known macromolecular target
  - v. Computational assessment of activity and toxicity and drugability.

**References:**

1. **Leach, A. R.; Gillet, V. J. (2007), An introduction to Chemoinformatics, Springer.**
2. **Gasteiger, J.; Engel, T. (2003), Chemoinformatics: A text-book. Wiley-VCH.**
3. **Gupta, S. P. (2011), QSAR & Molecular Modeling. Anamaya Pub.**
4. **Gasteiger, J. Handbook of cheminformatics: from data to knowledge in 4 volumes, Wiley.**

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## DISCIPLINE SPECIFIC ELECTIVE10

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>CHEMICAL PATENT ANALYTICS &amp; IP STRATEGY</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>-</b>

#### Course Objectives:

- Develop expertise in chemical patent analysis, drafting, and intellectual property (IP) strategy.
- Provide hands-on training in patent search methodologies, analytics, and database navigation.
- Foster understanding of IP commercialization, technology transfer, and portfolio management in the chemical industry.

#### Learning Outcomes:

By the end of this course, students will be able to learn:

- Analyze chemical patent systems, including Indian and global frameworks (USPTO, EPO, PCT).
- Conduct patent searches, patentability, freedom-to-operate (FTO) analyses, and landscape studies using AI and databases.
- Draft patent claims, specifications, and drawings for chemical inventions.
- Apply IP strategies for commercialization, licensing, and competitive intelligence.

### THEORY COMPONENT-

#### UNIT 1: Chemical Patent Fundamentals

(8 Hours)

**Introduction to Chemical Patents:** Anatomy of patent: Patent number, inventors, assignee, dates, title, abstract, background, summary, claims, description, drawing, embodiment, etc. Types of chemical patents: Composition, process, formulation, use patents, special considerations for biotechnology patents, differences between product and process patents in chemistry

**Indian Patent System for Chemicals:** Section 3(d) and its implications for pharma patents, compulsory licensing case studies (Bayer vs Natco), traditional knowledge protection (Turmeric, Neem cases)

**Global Patent Systems:** PCT filing for chemical inventions, USPTO and EPO requirements for chemical patents, Patent term extensions for agrochemicals

**Patentability Criteria:** Novelty assessment for chemical compounds, inventive step in process chemistry, industrial applicability requirements

## **UNIT 2: Patent Search & Analysis**

**(8 Hours)**

**Search Methodologies:** Keyword strategies for chemical searches, classification systems (IPC, CPC for chemistry), structure-based searching (Markush, SMILES, InChI)

**Database Navigation:** WIPO Patentscope deep dive, USPTO chemical patent search techniques, specialized chemistry databases (SciFinder, Reaxys), Google patent, Lens.org, FreePatentOnline, Derwent Innovation, PatSnap, Orbit Intelligence (Questel), PatBase, Reaxys, and SciFinder

**Analytical Techniques:** Citation analysis for identifying key patents, patent family mapping, competitive intelligence through assignee analysis

**Freedom-to-Operate Analysis:** Risk assessment methodology, case study: generic drug entry strategies

## **UNIT 3: Patent Drafting for Chemists**

**(8 Hours)**

**Claim Drafting Strategies:** Composition claims vs process claims, Markush language for chemical structures, dependent claim strategies

**Specification Writing:** Detailed description requirements, examples and embodiments, data presentation best practices

**Special Cases:** Polymorph patents, formulation patents, biotech sequence listings

**Drawings and Diagrams:** Chemical structure drawings, Process flow diagrams, spectra presentation

## **UNIT 4: IP Commercialization**

**(6 Hours)**

**Technology Transfer:** University-industry collaborations, licensing strategies, startup formation

**Portfolio Management:** Patent valuation methods, maintenance decision making, defensive publishing, case **Studies:** Novartis Glivec case, agrochemical patent strategies. green chemistry patents,

## **PRACTICAL COMPONENT**

**(60 Hours)**

### **1. Basic Excel Training (May use AI tools as well)**

Essential formulas:

VLOOKUP (for patent family matching)

COUNTIF (for assignee analysis)

Pivot Tables (for technology trend analysis)

Conditional Formatting (highlighting key patents)

Data cleaning techniques for patent exports

### **2. Database Navigation and Export**

WIPO Patentscope, USPTO, Espacenet, Google Patent, Lens.org, FreePatentsOnline

Non-Patent Literature data bases (Google Scholar, Science direct, Scopus, Scopus AI)

### **3. Novelty Search (Invention from any recent patent application)**

Task: Identify prior art for a given invention

Tools: Any freely available data base including AI tools

Deliverable: Excel report with key patents ranked by relevance and novelty assessment summary

**5. FTO Search** (Provide an invention from any recent granted patent)

Task: Analyze freedom-to-operate for a provided invention

Tools: Any freely available data base including AI tools

**Deliverable:** Risk assessment matrix in Excel

**6. Invalidity Search** (Provide a recent granted patent)

Task: Find invalidating prior art for a granted patent

Tools: Any freely available data base including AI tools

Deliverable: Evidence chart in Excel

**7.Claim Drafting** (Provide an Invention disclosure from a patent)

**8. Group project + viva presentation on landscape study**

Task: Any topic in a particular interval (2020 to 2025) and convert landscape study into PowerPoint

Tools: Any freely available data base including AI tools, excel, and PPT

Deliverable: Pivot table showing: Top assignees and Technology evolution

Requirements: Technology trends slides, competitor analysis.

## RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

1. WIPO, WIPO Patent Drafting Manual (2023) – World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-867-23-en-wipo-patent-drafting-manual.pdf>)
2. Sampat BN, Shadlen KC. Indian pharmaceutical patent prosecution: The changing role of Section 3(d). PLoS One. 2018 Apr 2;13(4):e0194714. doi: 10.1371/journal.pone.0194714. PMID: 29608604; PMCID: PMC5880378.
3. WIPO, Guidelines for Preparing Patent Landscape Reports(2015)-World Intellectual Property Organization ([https://www.wipo.int/edocs/pubdocs/en/wipo\\_pub\\_946.pdf](https://www.wipo.int/edocs/pubdocs/en/wipo_pub_946.pdf))
4. WIPO, Patent Cooperation Treaty(PCT)- Regulations under the PCT (as in force from July 1, 2024) (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-274-2024-en-patent-cooperation-treaty-pct.pdf>)
5. WIPO, Guide to the International Patent Classification (2025)-World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-guide-ipc-2025-en-guide-to-the-international-patent-classification-2025.pdf>)
6. WIPO, Inventing the Future-An Introduction to Patents for Small and Medium-sized Enterprises (2018)-World Intellectual Property Organization (<https://www.wipo.int/edocs/pubdocs/en/wipo-pub-917-1-en-inventing-the-future.pdf>)
7. WIPO, Identifying Inventions in the Public Domain-A Guide for Inventors and Entrepreneurs (2020)-World Intellectual Property Organization ([https://www.wipo.int/edocs/pubdocs/en/wipo\\_pub\\_1062.pdf](https://www.wipo.int/edocs/pubdocs/en/wipo_pub_1062.pdf))
8. <https://www.uspto.gov/patents/basics>

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## DISCIPLINE SPECIFIC ELECTIVE11

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
FUNDAMENTALS OF MEDICINAL CHEMISTRY	4	2	0	2	12 <sup>th</sup> Class: Physics, Chemistry, Mathematics	-

**\*\*For syllabus content of Discipline Specific Elective-11: (DSE-11) “Fundamentals of Medicinal Chemistry” refer to the syllabus content of DSE-20 of B Sc. Physical Sciences Programme.**

## GENERIC ELECTIVE

### CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
<b>INDUSTRIAL POLLUTION-IMPACTS&amp; REMIDIES</b>	<b>4</b>	<b>2</b>	<b>0</b>	<b>2</b>	<b>12<sup>th</sup> Class: Physics, Chemistry, Mathematics</b>	<b>-</b>

#### Course Objectives

- To understand the sources, types, and impacts of industrial and environmental pollutants.
- Study remediation techniques and sustainable practices for pollution control.
- Develop hands-on skills for pollutant analysis using non-sophisticated methods.
- Analyze case studies of environmental disasters and policy responses.

#### Learning Outcomes

By the end of the course, students will be able to:

- Classify major pollutants (air, water, soil) and describe their environmental pathways.
- Explain the chemistry behind pollution effects (e.g., acid rain, bio-magnification).
- Perform basic pollutant detection and remediation experiments.
- Evaluate Indian and global environmental regulations (CPCB, NGT, Paris Agreement).
- Propose sustainable solutions using green chemistry principles.

### THEORY COMPONENT

#### Unit 1: Fundamentals of PollutionTypes (8 Hours)

- **Types of Pollution:** Air, water, soil, noise, thermal - definitions, key features, and examples from urban and industrial settings.
- **Pollutant Classification:** Organic pollutants (e.g., volatile organic compounds, pesticides, PAHs), inorganic pollutants (e.g., heavy metals, acids, ammonia), and particulate matter (PM<sub>2.5</sub>, PM<sub>10</sub>).
- **Sources of Pollution:** Natural vs. anthropogenic; emissions from chemical industries, fossil fuel combustion, mining operations, fertilizer and pesticide use, and urban waste.
- **Environmental Pathways:** Introduction to pollutant transport and fate — atmospheric deposition, leaching into groundwater, surface runoff, bioaccumulation, and biomagnification in food chains.



## Unit 2: Impacts and Monitoring (7 Hours)

- **Health Effects of Pollutants:** Acute and chronic impacts — respiratory diseases, carcinogenicity (benzene, dioxins), neurotoxicity (lead, mercury), endocrine disruption.
- **Ecosystem Damage:** Eutrophication of water bodies, degradation of soil fertility, deforestation, and loss of biodiversity.
- **Climate Linkages:** Role of CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O in global warming; CFCs and ozone layer depletion; interconnections between local pollution and global environmental change.
- **Case Studies:**
  - Bhopal Gas Tragedy (1984): Methyl isocyanate release and its aftermath
  - Minamata Disease (Japan): Industrial mercury poisoning

## Unit 3: Environmental Laws & Policies (7 Hours)

- **Indian Regulations:**
  - Water (Prevention and Control of Pollution) Act, 1974
  - Air (Prevention and Control of Pollution) Act, 1981
  - Environment Protection Act (EPA), 1986
  - Role of the National Green Tribunal (NGT) in enforcement
- **Global Frameworks:**
  - Kyoto Protocol: Binding targets for developed nations
  - Paris Agreement: Global commitment to climate mitigation
- **Monitoring Techniques:**
  - Air: *AQI metrics, stack emission sampling, ambient air samplers*
  - Water: *Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD), heavy metal testing, TDS*
  - Soil: *pH, electrical conductivity, nutrient levels, contaminant profiling (e.g., lead, arsenic)*

## Unit 4: Remediation & Sustainability (8 Hours)

- **Remediation Techniques:**
  - Physical Methods:* Filtration, adsorption using activated charcoal, sedimentation
  - Chemical Methods:* Precipitation of heavy metals, neutralization of acid/alkali wastes, oxidation-reduction methods
  - Biological Methods:* Bioremediation (microbial degradation), phytoremediation (use of plants like *Brassica*, *Eichhornia*)
- **Green Chemistry Approaches:** 12 principles of green chemistry, pollution prevention at the source, eco-friendly solvents, catalysis, energy-efficient synthesis
- **Circular Economy Concepts:** Resource reuse, closed-loop systems, industrial symbiosis, cradle-to-cradle design
- **Corporate Environmental Responsibility:**
  - CSR initiatives in environmental conservation
  - Zero-liquid discharge (ZLD) in process industries
  - Extended Producer Responsibility (EPR) in plastic and electronics sectors

## PRACTICAL COMPONENT (60 hours)

1. pH and acidity testing of effluents (comparison of household and industrial acids)
2. Test for coagulation-flocculation (alum treatment of turbid water)

3. Qualitative detection of heavy metals (lead/iron) using sodium sulfide
4. Dissolved oxygen estimation using Winkler's method
5. Soil salinity test using conductivity meter
6. Colorimetric adsorption study (methylene blue on charcoal or silica)
7. Noise pollution mapping using smartphone dB meters in campus zones
8. Airborne particulate capture using sticky tapes and microscopic analysis
9. Neutralization experiments with acidic waste (lime, baking soda titration)
10. Oil–water separation using charcoal/cotton filters.

## RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

### Textbooks:

De, A. K., *Environmental Chemistry* – New Age International.  
 Manivasakam, N., *Industrial Pollution Control* – SS Publishers.  
 Anastas, P. T., & Warner, J. C., *Green Chemistry: Theory and Practice* – Oxford University Press.  
 Pepper, I. L., Gerba, C. P., & Brusseau, M. L., *Pollution Science* – Academic Press.  
 Walker, P., & Wood, E., *Environmental Science Experiments* – Facts on File.  
 Thomas, W. J., *Adsorption Technology & Design* – Butterworth-Heinemann.  
 Smith, K. A., & Mullins, C. E., *Soil and Environmental Analysis* – CRC Press.  
 Skoog, D. A., West, D. M., Holler, F. J., & Crouch, S. R., *Fundamentals of Analytical Chemistry* (9th Edition) – Cengage Learning.  
 Vogel, A. I., Svehla, G., Jeffery, G. H., & Mendham, J., *Vogel's Qualitative Inorganic Analysis* (7th Edition) – Pearson.  
 Vowles, P. D., & Connell, D. W., *Experiments in Environmental Chemistry* – Elsevier.  
 Boyd, C. E., *Water Quality: An Introduction* – Springer.

### Reports & Guidelines:

- CPCB (Central Pollution Control Board) publications.
- UNEP (United Nations Environment Programme) reports.

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