# M.Sc. CHEMISTRY

## INORGANIC CHEMISTRY SPECIALISATION
## SYLLABUS OF III & IV SEMESTERS
## *REVISED AS PER NEW (CB) SYLLABUS*

## FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

## Osmania University

**M.Sc. Chemistry (Inorganic Chemistry) III and IV Semesters Programme**
**(For the batch admitted during the academic year 2016-2017 under the CBCS pattern)**
***[Under Restructured CBCS Scheme]***

# M.Sc. CHEMISTRY (INORGANIC CHEMISTRY SPECIALISATION)

## Syllabus for III and IV Semesters

**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

***[Under Restructured CBCS Scheme]***

***Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits***

**(Approved in the P.G. BOS meeting held on 01-07-2017)**

## Semester - III (Inorganic Chemistry)

## *[Under CBCS Scheme]*

**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

| | Hrs/week | Internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH(IC)301T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)302T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)303T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)304T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)351P (LAB-I) | 9 | | | 100 marks | 4 |
| CH(IC)352P (LAB-II) | 9 | | | 100 marks | 4 |
| **Total** | | | | **600 marks** | **24** |

## Semester - IV (Inorganic Chemistry)

| | Hrs/week | Internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH(IC)401T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)402T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)403T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)404T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(IC)451P (LAB-I) | 9 | | | 100 marks | 4 |
| CH(IC)452P (LAB-II) | 9 | | | 100 marks | 4 |
| **Total** | | | | **600 marks** | **24** |

## Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits

| | III Semester | | | |
|---|---|---|---|---|
| | **Course** | **Hours** | **Credits** | **Marks** |
| CORE | **Paper-I: CH(IC)301T: Bonding, Group Theory and its Applications**<br>IC-09: Group Theory, Normal mode analysis and Spectral Activity<br>IC-10: MOT of Metal Complexes<br>IC-11: Electronic Spectroscopy of Metal Complexes<br>IC-12: IR and Raman Spectroscopy | 4 | 4 | 100 |
| CORE: | **Paper-II: CH(IC) 302T: Organo Metallic Chemistry of Transition Metal Complexes**<br>IC-13: Mono,Di and Trihapto Complexes<br>IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes<br>IC-15: Catalytic Role of OTMC-I<br>IC-16: Catalytic Role of OTMC-II | 4 | 4 | 100 |
| ELECTIVE IIIa | **Paper-III: CH(IC) 303T: Analytical Techniques-I**<br>IC-17: Data Handling<br>IC-18: AAS, AES, ICP-AES<br>IC-19: Diffraction Methods<br>IC-20: Advanced Mass spectrometry | 4 | 4 | 100 |
| ELECTIVE IIIb | **Paper-III: CH(IC) 303T: Supramolecular Chemistry, Photochemistry, Green Chemistry and Nanotechnology**<br>IC-21: Supramolecular Chemistry<br>IC-22: Photochemistry of Metal Complexes<br>IC-23: Green Chemistry<br>IC-24: Nanotechnology | 4 | 4 | 100 |
| ELECTIVE IVa | **Paper-IV:CH(IC) 304T: Analytical Techniques-II**<br>IC-25: Thermal Methods<br>IC-26: Surface Analysis Methods/ Microscopic analysis<br>IC-27: Advanced Separation Techniques<br>IC-28: Optical Methods | 4 | 4 | 100 |
| ELECTIVE IVb | **Paper-IV: CH(IC) 304T: Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry**<br>IC-29: Nuclear Chemistry<br>IC-30: Zeolites and Molecular Sieves<br>IC-31: Solid State Chemistry<br>IC-32: Surface Chemistry & Superconductors | 4 | 4 | 100 |
| LABORATORY COURSE -I | **CH (IC) 351P: Synthesis and Characterization of Metal Complexes** | 9 | 4 | 100 |
| LABORATORY COURSE –II | **CH (IC) 352P: Electro-Analytical techniques** | 9 | 4 | 100 |

| | IV Semester | | | |
|---|---|---|---|---|
| | **Course** | **Hours** | **Credits** | **Marks** |
| CORE | **Paper-I: CH(IC)401T: Molecular Spectroscopy of Inorganic Compounds**<br>IC-33: Multinuclear NMR<br>IC-34: Advanced NMR techniques<br>IC-35:Applications of ESR to Metal Complexes<br>IC-36:Mossbauer Spectroscopy and Nuclear Quadrupole Resonance Spectroscopy | 4 | 4 | 100 |
| CORE | **Paper-II: CH(IC) 402T: Bioinorganic Chemistry**<br>IC-37: Metal ions Interactions with Nucleic acids and their constituents.<br>IC-38: Transport of Electrons and Metal ions.<br>IC-39: Metallo-Enzymes of Iron, Zinc and Nickel.<br>IC-40:Metallo-Enzymes of Cobalt, Copper Molybdenumand Manganese | 4 | 4 | 100 |
| ELECTIVE IIIa | **Paper-III: CH(IC)403T: Medicinal Inorganic Chemistry, Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials**<br>IC-41: Metal complexes in Clinical Chemistry<br>IC-42:Metal complexes as Drugs and Anticancer agents<br>IC-43:Spectroscopic analysis of drug/metal complexes binding to DNA<br>IC-44: Applications of Nanomaterials | 4 | 4 | 100 |
| ELECTIVE IIIb | **Paper-III:CH(IC)403T:Analytical Techniques-III**<br>IC-45: Electroanalytical Methods<br>IC-46: Radiochemical Methods<br>IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry<br>IC-48: Industrial Analysis | 4 | 4 | 100 |
| ELECTIVE IVa **(ID Paper)** | **Paper-IV: CH(ID) 404T: Interdisciplinary Course (Environmental and Applied Analysis)**<br>IC-49 : Clinical and Pharmaceutical Analysis<br>IC-50: Food and Agricultural analysis<br>IC-51: Analysis of Air and Water Pollutants<br>IC-52: Drinking Water and Sewage Water Treatment | 4 | 4 | 100 |
| ELECTIVE IVb **(ID Paper)** | **Paper-IV: CH(ID) 404T: Interdisciplinary Course (Inorganic Material Chemistry)**<br>IC-49 : Composite Materials<br>IC-50: Liquid Crystals<br>IC-51: Explosives and Propellants<br>IC-52: Fuels and Combustion | 4 | 4 | 100 |
| LABORATORY COURSE –I | **CH (IC) 451P: Conventional Methods of Analysis** | 9 | 4 | 100 |
| LABORATORY COURSE –II | **CH (IC) 452P: Spectroscopic Techniques** | 9 | 4 | 100 |

# M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
# SEMESTER-III
# PAPER I

## CH(IC)301T: Bonding Group Theory and its Applications

**IC-09: Group Theory, Normal mode analysis and Spectral Activity**
**IC-10: MOT of Metal Complexes**
**IC-11: Electronic Spectroscopy of Metal Complexes**
**IC-12: IR and Raman Spectroscopy**

## Course Objectives

1. Learn group theory basics in chemistry. Apply group theory to analyze vibrational modes. Connect group theory to spectral activity.
2. Understand MOT for metal complexes. Analyze electronic structures using MOT. Predict properties and reactivity with MOT.
3. Learn principles of electronic transitions. Interpret electronic spectra. Study metal complexes using spectroscopy.
4. Understand IR and Raman spectroscopy principles. Analyze vibrational spectra. Apply spectroscopy to chemical analysis.

## Learning Outcomes

1. Students will be able to classify molecules by symmetry. Identify vibrational modes using group theory. Predict and interpret IR and Raman spectra.
2. Students will be able to construct molecular orbital diagrams. Analyze electronic configurations and bonding. Predict reactivity and stability of metal complexes.
3. Students will be able to explain electronic transitions in metal complexes. Interpret UV-Vis spectra. Correlate spectral data with molecular properties.
4. Students will be able to understand principles of IR and Raman spectroscopy. Identify molecular vibrations from spectra. Apply spectroscopy for chemical analysis.

**IC-09: Group Theory, Normal Mode Analysis and Spectral Activity**

Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, salient features about Classes, Classes of $C_{2V}$, $C_{2h}$ and $C_{3V}$. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of $E$, $C_n$, $S_n$, i and σ Elements. Great Orhogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for $C_{2V}$, $C_{2h}$ and $C_{3V}$. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula.
Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for IR and Raman activity. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for $C_{2V}$ (eg. $H_2O$, $SF_4$), $C_3V$ ($NH_3$, $POCl_3$), $C_{2h}$ (trans-$N_2F_2$), $D_{3h}$ ($BF_3$), Td($SO_4^{2-}$), Oh ($SF_6$). Internal coordinate method of analysis for $C_{2V}$ ($H_2O$), $C_3V$ ($NH_3$), Td ($SO_4^{2-}$).

**IC-10: Molecular Orbital Theory of Metal Complexes:** Limitations of Crystal Field Theory, Adjustments to the Crystal Field Theory to allow for covalence -Experimental evidences for Metal -

Ligand orbital overlap. The Adjusted Crystal Field Theory. Introduction to Molecular Orbital Theory. Symmetry Classification of Metal and Ligand Group Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, TrigonalBipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams -Octahedral Metal Complexes with (i) Sigma (σ), (ii) sigma(σ) &Pi (π) and (iii) sigma (σ), Pi (π) and Pi* (π*) bonding contribution from the Ligands - Tetrahedral Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π), and Square Planar Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π) bonding contribution from the ligands - Molecular orbital electron configurations and calculation of Magnetic Moments.

**IC-11: Electronic Spectroscopy of Metal Complexes**

Classification of Electronic Spectra for Metal Complexes, Selection Rules: Electric Dipole Transitions, Magnetic Dipole Transitions, Orbital Selection Rules, Spin Selection Rules, Relaxation in Selection Rules. Nature of Electronic Spectral Bands: Band Widths, Band Intensities. Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series, Nephelauxetic Effect. Orgel Diagrams for $d^1$-$d^9$ Configurations, Crystal Field Spectra of $O_h$ and $T_d$ Metal Complexes of 3d Metals. Charge Transfer Spectra. Strong Field Configurations: The Method of Descending Symmetry, Correlation Diagrams and Tanabe-Sugano Diagrams for $d^2$ and $d^8$ Configurations. Calculation of 10Dq Values, Racah Parameter (B) and Nephelauxetic Ratio (β).

**IC-12: Infrared and Raman Spectroscopy**

Conditions for Infrared and Raman Spectroscopies, Direct product – symmetry requirements for overtones, binary and ternary combination bands. Partial Normal mode analysis-Structure Fitting, Determination of Coordination Sites and Linkage Isomers($NO_2^-$ , $SCN^-$), Assigning Denticity of Ligands ($SO_4^{2-}$, $CO_3^{2-}$), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Nitrogen, Carbon and Halogen Donors ($NH_3$, $H_2O$, Glycine, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, $CO_2$, $N_2O$, $H_2O$. Principles of Resonance Raman Spectroscopy. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers

**SUGGESTED BOOKS**


1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
11. Infrared spectroscopy of Inorganic Compound, Bellamy.


# PAPER II

## CH(IC) 302T: Organo Metallic Chemistry of Transition Metal Complexes

**IC-13: Mono,Di and Trihapto Complexes**
**IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes**
**IC-15: Catalytic Role of OTMC-I**
**IC-16: Catalytic Role of OTMC-II**

## Course Objectives

1. Understand the bonding in mono-, di-, and trihapto complexes. Analyze the structure and stability of these complexes. Explore the reactivity and applications of mono-, di-, and trihapto complexes.
2. Learn the bonding and structure of multi-hapto complexes. Examine the stability and electronic properties of these complexes. Investigate the reactivity and applications of tetra-, penta-, hexa-, hepta-, and octahapto complexes.
3. Understand the catalytic mechanisms of organotransition metal complexes (OTMC). Analyze the factors influencing catalytic activity in OTMC-I. Explore applications of OTMC-I in industrial processes.
4. Study advanced catalytic mechanisms of OTMC. Evaluate the factors affecting catalytic performance in OTMC-II. Investigate the applications of OTMC-II in advanced industrial processes.

## Learning Outcomes

1. Students will be able to Identify bonding in mono-, di-, and trihapto complexes. Analyze structure and stability. Understand reactivity and applications.
2. Students will be able to Identify bonding in multi-hapto complexes. Examine stability and electronic properties. Understand reactivity and applications.
3. Students will be able to understand catalytic mechanisms of OTMC-I. Analyze factors influencing catalytic activity. Explore industrial applications.
4. Study advanced catalytic mechanisms of OTMC-II. Evaluate factors affecting catalytic performance. Investigate advanced industrial applications.

**IC-13: Mono, Di and Tri hapto Complexes**

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand. 16 and 18 electron rules. Electron countingcovalentand ionic models. $\eta^1$ – Complexes : General methods of Preparation –Bonding of Ligand to Metal :αand βInteraction and agostic interaction– Stability and decomposition pathways –$\eta^1$ Complexes –Tertiary Phosphine – Transition Metal Alkyl and Aryl Complexes of Pt – Ortho-effect – Bonding in Metal – Carbene and Carbyne Complexes. $\eta^2$ –Complexes: General methods of preparation of Metal – Alkene Complexes – Structure and Bonding in $\eta^2$ Complexes-Zeises salt – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes: Metal-Allyl Complexes – General Preparative Routes – Structure and Bonding in η3 Allyl Complexes – Fluxionality.

**IC-14: Tetra, Penta,Hexa,Hepta and Octahapto Complexes**

η4 Complexes: Structure and Bonding in η4 Complexes –Butadiene and Cyclobutadiene Complexes. η5 – Complexes: General methods of Preparation – Bis (η5-cyclopentadienyl) metal complexes (Metallocenes) – Ferrocene: Structure and Bonding –Reactions of Ferrocene – Mechanism of Electroplilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions.

$\eta^6$Complexes : Metal –Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding in Bis(arene)-Metal Complexes – Reactions. $\eta^7$Complexes : Preparation , Structure and Reactions of $\eta^7$ – $C_7H_7$ Complexes. $\eta^8$Complexes : $C_8H_8$ as a Ligand – Cyclooctatetraene Complexes – Preparation, Structure and Bonding in Uranocene.

**IC-15: Catalytic Role of OTMC-I**

Oxidative addition and Reductive Elimination : Stereochemistry and Mechanism of Oxidative Addition – Insertion Reactions – Hydrogenation of Olefins –Transfer Hydrogenation –Hydrosilation of Olefins – Isomerisation of Olefins – Ziegler –Natta Polymerization of Olefins – Oligomerization of Butadiene Alkene Metathesis. Dupont-1,4-hexadiene synthesis.Oxidation of Olefins to Carbonyl Compounds – Oxidation of Hydrocarbons to Alcohols and Acids – Oxidation of Aldehydes, Cyclohexanol, Cyclohexanone, p-Xylene.

**IC-16: Catalytic Role of OTMC- II**

Reactions of Carbon monoxide and Hydrogen:Hydroformylation – Carbonylation –Syngas- Water gas shift Reaction (WGS) – Reactions of Syngas. Applications of Metal Clusters in Catalysis:Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$ – , Hydrogenation of Olefins. Use of $[Fe_4C(CO)14]$ as a model for Fischer – Tropsch process. Recent Developments in Homogenous Catalysis: Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under Phase Transfer Conditions: Hydrogenation. Bio Catalysis : Enzyme Analogue Catalysis: Introduction, Examples of Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, Metal Cations as Templates, Covalent molecules as Templates, External and Internal Templates – Homogeneous Catalysts and their Heterogenization or Immobilization by Aqueous Catalysis.

**SUGGESTED BOOKS**


1.Organometallics-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH

2.Organotransition Metal Chemistry Fundamental Concepts and Applications, John AkioYamamato, Wiley & Sons.

3.Homogeneous Catalysis by Metal Complexes, M MTaqui Khan and A E Martel

4. Applied Homogenous Catalysis with Organo Metallic Compounds Vol I & II, Boy Cornillsand W A Herrmann – VCH

5. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II

6. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed

7. Symmetry and spectroscopy, K Veera Reddy

8. Homogenous catalysis, G W Parshall, John Wiley & Sons, New York

9. Basic organometallic Chemistry, B.D. Gupta / A. J. Elias

# PAPER III

## CH(IC) 303T ( Elective IIIa ): Analytical Techniques - I

**IC-17: Data Handling**
**IC-18: AAS, AES, ICP-AES**
**IC-19: Diffraction Methods**
**IC-20: Advanced Mass spectrometry**

## Course Objectives

1. Learn data collection and processing techniques. Apply statistical methods for data analysis. Interpret and present scientific data effectively.
2. Understand principles of AAS, AES, and ICP-AES. Learn instrumentation and methodologies. Apply these techniques for elemental analysis.
3. Understand the principles of diffraction. Learn techniques like X-ray, neutron, and electron diffraction. Apply diffraction methods to determine molecular structures.
4. Understand advanced mass spectrometry principles. Learn about various mass analyzers and ionization techniques. Apply mass spectrometry for complex molecular analysis.

## Learning Outcomes

1. Students will be able to collect and process scientific data. Analyze data using statistical methods. Interpret and present data effectively.
2. Students will be able to understand AAS, AES, and ICP-AES principles. Use relevant instrumentation and techniques. Conduct elemental analysis using these methods.
3. Students will be able to comprehend principles of diffraction. Apply X-ray, neutron, and electron diffraction techniques. Determine molecular structures using diffraction methods.
4. Students will be able to understand advanced mass spectrometry concepts. Use various mass analyzers and ionization techniques. Analyze complex molecules with mass spectrometry.

**IC-17: Data Handling**

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data ( mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.

**IC-18: AAS, AES, ICP-AES**

**Atomic Absorption Spectroscopy (AAS):** Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences –chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.

**Atomic Emission Spectroscopy (AES):** Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.

**Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES):** Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.
**Flame Photometry:** Principle, Theory, Instrumentation and Applications

**IC-19: Diffraction Methods**
X – ray Diffraction : X –rays and their generation – choice of radiation ; Miller indices, Braggs equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X – rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkylbiphosphate ; Advantages and limitations of X – ray Diffraction.
Electron Diffraction by gases :Principles , Radial distribution curves- Interpretation of results for $PBrF_2S$, $PF_3S$, $PF_2HS$, $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and $HgCl_2$ molecules, Advantages and Limitations
Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, Advantages and limitations.

## IC-20: Advanced Mass spectrometry
**Mass Analyzers**: Quadruple, Ion traps, Time of flight (TOF) mass analyzers
**Mass Spectrometry / Mass Spectrometry**: Tandem Mass Spectrometry, Instrumentation, Applications.
**Hyphenated Techniques: GC-MS** Principle, instrumentation, Interfaces- Direct coupling interface and open split interface. Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine. **LC-MS-** principle, Instrumentation – Interfaces- Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionization interface.**ICP – MS** - Principle Instrumentation, and Applications.
**Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry (MALDI-TOF-MS)**: Principle, Matrix, Sample Preparation for MALDI-MS - Dried droplet Crystallization, Thin layer method, Sandwich Crystallization, Instrumentation, Applications

**SUGGESTED BOOKS**


1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York.
2. Instrumental Methods of Chemical Analysis, H. Kaur.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson EducationLtd.
4. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
5. Instrumental Techniques for Analytical Chemistry, Frank Settle.
6. Principles of Analytical Chemistry, M. Valcarcel.
7. Solid State Chemistry and its Applications, *West.*
8. Introduction to Solids, Azaroff.
9. Solid State Chemistry, D.K. Chakrabarthy
10. Physical Methods in Advanced Inorganic Chemistry, Hill and Day.
11. Instrumental Methods of Analysis, Sixth edition, CBS Publishers, Willard, Merrit, Dean,and Settle.
12. Mass spectrometry for Chemists and Biochemists, Robert A.W Johnstone and Molcolm. E.Rose, second Edn.
13. Physical methods for Chemists, Russell S. Drago second edition, Saunders Collegepublishing 1992.
14. Structural methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H Rankin and S.Craddeck, ELBS.
15. Mass Spectrometry Basics, Herbert, Christopher G.; Johnstone, Robert A.W., CRC Press.
16. Mass Spectrometry-A Textbook by Jürgen H. Gross, © Springer-Verlag Berlin Heidelberg 2004, Printed in Germany.
17. Matrix-assisted laser desorption/ionization - https://en.wikipedia.org/wiki/Matrix-assisted_laser_desorption/ionization

# PAPER III

## CH(IC) 303T ( Elective IIIb ): Supramolecular Chemistry, Photochemistry, Green Chemistry and Nanotechnology

**IC-21: Supramolecular Chemistry**
**IC-22: Photochemistry of Metal Complexes**
**IC-23: Green Chemistry**
**IC-24: Nanotechnology**

## Course Objectives

1. Understand principles of supramolecular chemistry. Explore host-guest interactions and self-assembly. Analyze applications in materials and biological systems.
2. Learn the fundamentals of photochemistry in metal complexes. Study photophysical and photochemical processes.Investigate applications in catalysis and materials science.
3. Understand the principles of green chemistry. Develop sustainable chemical processes. Apply green chemistry concepts in industry and research.
4. Learn the basics of nanotechnology. Explore the synthesis and characterization of nanomaterials. Investigate applications in electronics, medicine, and materials science.

## Learning Outcomes

1. Students will be able to understand supramolecular chemistry principles. Analyze host-guest interactions and self-assembly. Apply concepts to materials and biological systems.
2. Students will be able to comprehend photochemistry of metal complexes. Study photophysical and photochemical processes. Investigate applications in catalysis and materials science.
3. Students will be able to understand green chemistry principles. Develop sustainable chemical processes. Apply green chemistry in industry and research.
4. Students will be able to understand nanotechnology fundamentals. Explore synthesis and characterization of nanomaterials. Apply nanotechnology in electronics, medicine, and materials science.

**IC-21: Supramolecular Chemistry**

**Host – Guest chemistry:** Definition and different types of host and guests with examples – types of non-covalent interactions – binding constants of host guest complex and thermo dynamics involved in it – designing principles of host.

**Cation guest binding** – binding between metal cations and macro cycles – chelate and cryptate effects – relationship between cavity size of host and cation radius and stability of resultant complexes – binding of macro cycles having secondary binding sites.

**Anion guest binding** – different hosts for anionic guests capable of binding through electro static interactions, hydrogen bonds, lewis acidic hosts – enhancement of binding strength using more than non-covalent interactions.

**Neutral guest binding –** binding of neutral guest using hydrogen bonding, $\pi$ - $\pi$ stacking, hydrophobic effect and charge transfer interactions – simultaneous binding of cation and anion guests – cascade approach, individual binding sites and zwitter ions approach –present and future applications – phase transfer agents – separation of mixtures – molecular sensors – switches and molecular machinery.

**IC-22: Photochemistry of Metal Complexes**

Energy, Structure, Electron Distribution and Chemical reactivity of Electronically Excited states of Coordination Compounds. Photochemistry of Cr(III) and Co(III) metal complexes . Photochemistry of $Cr(CO)6$ ,$Mn_2(CO)_{10}$ and $Fe(CO)_5$.

Structuredphosphorescence of Ruthenium Bipyridyl and Ortho-phenanthroline Complexes. Energy transfer Spin Correlation energy levels in the energy Transfer Systems;$[Ru(bipy)_3]^{2+}$ $[Cr(CN)_6]^{3-}$. Metal Sensitizers and Quenchers - Electron Relay. Photochemical Hydrogen production by oxidative quenching of $[Ru(bipy)_3]^{2+*}$ by Methyl Viologen.

**IC-23: Green Chemistry**

Principles and concepts of green chemistry

Introduction, sustainable development and green chemistry, atom economy, atom economic reactions, rearrangement reactions, addition reactions, atom uneconomic reactions- substitution reactions, elimination reactions, Wittig reactions. Reducing toxicity, measuring toxicity.

Organic solvents: Environmentally benign solutions: Organic solvents and volatile organic compounds, solvent free systems, super critical fluids- supercritical carbon dioxide and supercritical water. Water as a reagent solvent, water based coatings.

Industrial case studies: A brighter shade of green – greening of acetic acid, Vitamin C synthesis –enzyme routes. Polythene manufacture-metallocene catalysis.

## IC-24: Nanotechnology

**Metal Nanoclusters** –Introduction, Magic numbers, theoretical modeling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nanotransition.

**Methods of synthesis:** RF plasma, thermolysis, pulsed laser, chemical methods.

**Carbon nanostructures-** Introduction, carbon molecules, new carbon structures,

**Carbon clusters**- small carbon clusters, discovery of $C_{60}$, structure of $C_{60}$ and its crystal, alkali doped $C_{60}$, superconductivity in $C_{60}$.

**Carbon nanotubes:** Fabrication, structure, electrical properties, vibrational properties, mechanical properties.

**Nanophase and nanostructured materials**: **Micells and Microemulsions -** Formation mechanisms of micelles and microemulsions, the critical Micelle Concentration (CMC) for surfactants, Solubilization and Formation of Microemulsions. **Synthesis of Nanoparticles from W/O Microemulsions:** Preparation of Nanoparticles of Metals, Metal Sulfides, Metal Salts, Metal oxides, Nanowires. **Synthesis of Organic Nanoparticles from O/W Microemulsions:** Styrene Latex NanoParticles, Methylmethacrylate Nanoparticles. Sol -Gel process for the fabrication of Glassy and Ceramic materials.

**SUGGESTED BOOKS**


1. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn
2. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons
3. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
4. Concepts of Inorganic PhotoChemistry A.W. Adamson and P. D. Fleschaner,Wiley.
5. Inorganic Photochemistry, Journal of Chemical Education, Vol 60. No 10, 1983.
6. Progress in Inorganic Chemistry Vol 30 ed :S.J.Lippard.
7. Coordination Chemistry Reviews Vol 39 1981,p121
8. Photochemistry of Coordination compounds V.Balzani and Carassiti,academicpresss.
9. Elements of inorganic Photochemistry G.J.Ferrendi,Wiley,
10. Structure and Bonding Vol 49 1982.
11. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers, 1991.

12. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt CollegePublishers, 1998.
13. Analytical Chemistry - Gary Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition, 1994.
14.Green Chemistry- An Introductory text by Mike Lancaster- RSC.
15. Green Chemistry: Theory and Practice by John C. Warner Paul T. Anastas.
16. Introduction to nanotechnology by Charles P. Poole Jr, Frank J. Owens- Wiley StudentEdition 2006.
17. Hand Book of Nanophase Materials by A.N. Gold Stein ed,Marcel Decker, New York, 1997, Chapter1
18. Clusters of Transition Atoms" by Morse, Chem. Rev 86, 1049 (1986).
19. Hand Book of Nanostructured materials by P.M. Ajayan, H.S Nalwa, ed, AcademicPress, San Diego, 2000, Vol. 5, Chapter 6.
20. Hand Book of Nanophase and Nanostructured materials, volume I: Synthesis, Zhong Lin Wang, Yi Liu,Ze Zhang.

# PAPER IV

## CH(IC) 304T ( Elective IVa ): Analytical Techniques-II

**IC-25: Thermal Methods**
**IC-26: Surface Analysis Methods/ Microscopicanalysis**
**IC-27: Advanced Separation Techniques**
**IC-28: Optical Methods**

## Course Objectives

1. Understand principles of thermal analysis techniques. Learn methodologies like TGA, DSC, and DTA. Apply thermal methods to study material properties.
2. Understand principles of surface and microscopic analysis. Learn techniques like SEM, TEM, AFM, and XPS. Apply these methods for surface characterization.
3. Understand advanced separation principles. Learn techniques like HPLC, GC, and electrophoresis. Apply separation techniques in chemical analysis.
4. Understand principles of optical spectroscopy. Learn techniques like UV-Vis, IR, and fluorescence spectroscopy. Apply optical methods for molecular analysis.

## Learning Outcomes

1. Students will be able to understand thermal analysis principles. Utilize techniques like TGA, DSC, and DTA. Analyze material properties using thermal methods.
2. Students will be able to understand surface and microscopic analysis principles. Use techniques like SEM, TEM, AFM, and XPS. Characterize surfaces using these methods.

3. Students will be able to understand advanced separation techniques. Employ methods like HPLC, GC, and electrophoresis. Perform chemical analysis using separation techniques.
4. Students will be able to understand optical spectroscopy principles. Use techniques like UV-Vis, IR, and fluorescence spectroscopy. Analyze molecules using optical methods.

**IC-25: Thermal Methods**

**Thermogravimetric analysis (TGA)**: Principle, Instrumentation, working function of each component, applications of TGA, Study of oxalates, nitrates and chromates by TGA. Determination of carbon black in polythene.

**Differential thermal analysis (DTA)**: Principle, Instrumentation, Methodology, applications. Differential thermogram of sulphur. TG and DTA of manganese phosphine monohydrate.

**Differential scanning calorimetry (DSC)**: Principle, instrumentation, power compensated DSC instruments and Heat flow DSC instruments, Methodology, DSC experiment calibration and data analysis. Applications determination Glass transition temperatures and heat capacities, problems based on Thermal Techniques:

**Thermometric titrations**: Principle, apparatus, applications to acid base, precipitation, complexometric, redox and non-aqueous titrations.

**Combined thermal instruments**: Introduction to TGA/MS and TGA/FTIR, High resolution TGA, Microthermal analysis.

**IC-26: Surface Analysis Methods/ Microscopic analysis**

Introduction, types of surface measurements.

**Photon Probe Tecnhniques**: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.

**Electron Probe Techniques**: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Transmission Electron Microscopy (TEM) - Principle, Instrumentation, applications. Energy Dispersive X-ray Spectroscopy (EDX) - Principle, Instrumentation, applications. Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.

**Ion Probe Techniques**: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications

**Scanning probe microscopy Techniques**: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

**IC-27: Advanced Separation Techniques**

**Separations by extractions**: Solid phase extraction- Principle, methodology, applications. Solvent extraction of flow injection analysis. Applications to extractions of metal ions by chelating agents (Dithiazone, 8-hydroxy quinoline and cupferron). Organic reagents in Inorganic analysis - Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone, thionyl-trifluoroacetone, tri-n-octyl phosphine oxide.

**Affinity and chiral chromatography** – Principle, technique, Instrumentation and applications.

**Size Exclusion Chromatography** – Principles of gel – filtration Chromatography, Instrumentation, retention behavior, resolution, selection of gel type, applications, **Ion exclusion** – Principle and applications.

**Supercritical fluid chromatography (SFC)** – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.

**GC-FT-IR:** Instrumentation, Principles and Applications

**IC-28: Optical Methods**

**CD, ORD and Fluorescence:** Optical rotator dispersion and Circular dichorism: Principles - Optical rotation, circular birefringence, circular dichroism and Cotton effect, Octet Rule, Experimental Techniques, Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes. Theory and principles of fluorescence spectroscopy. Characteristic of fluorescence emission, Fluorescence life time, quantum yield, Static and dynamic/collisional quenching and comparison. Fluorescence polarization and polarization spectra of a fluorophore. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies

**SUGGESTED BOOKS**


1. Principles of Instrumental Analysis: Holler, Skoog and Ccrouch, 6th edition ,Cengage Learning 2007.
2. Instrumental methods of chemical analysis B.K. Sharma, Goel Publishing House.
3. Instrumental Methods of analysis, Willard Mersritt, Dean and Settle, 7th edition, CBS Publishers 1986.
4. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York 1994.
5. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
6. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA, 1997.
7. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed., Longmann, ELBS Publications, 2000.
8. Principles of fluorescence spectroscopes – Lakowicz.
9. Fluorescence Quenching theory and applications – Maurice R. Eftink.
10. Circular Dichroism Spectroscopes of DNA Methods in Enzymology Vol 211.
11. Tris (Phenanthroline) Metal complexes: probes for DNA Helicity Journal of Biomolecular structure and Dynamics Adenine Press 1983. G.L. Eichorn.8
12. Tris (Phenanthroline) Ru(II) Enantiomers interactions with DNA : Mode and specificity of binding J.B. Chaires. Biochemistry 1993 (32) 2573


# PAPER IV

## CH(IC) 304T ( Elective IVb ): Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry

**IC-29: Nuclear Chemistry**
**IC-30: Zeolites and Molecular Sieves**
**IC-31: Solid State Chemistry**
**IC-32: Surface Chemistry & Superconductors**

## Course Objectives

1. Understand the principles of nuclear chemistry. Study nuclear reactions and decay processes. Explore applications of nuclear chemistry in energy and medicine.
2. Learn about the structure and properties of zeolites and molecular sieves. Understand synthesis and characterization techniques. Explore applications in catalysis and separation processes.
3. Understand the principles of solid-state chemistry. Study crystal structures and bonding in solids. Explore the properties and applications of solid materials.
4. Understand the principles of surface chemistry. Study the properties and applications of superconductors. Explore techniques for surface characterization.

## Learning Outcomes

1. Students will be able to understand nuclear chemistry principles. Analyze nuclear reactions and decay processes. Explore applications in energy and medicine.
2. Students will be able to understand the structure and properties of zeolites and molecular sieves. Learn synthesis and characterization techniques. Apply these materials in catalysis and separation processes.
3. Students will be able to understand solid state chemistry principles. Analyze crystal structures and bonding in solids. Explore properties and applications of solid materials.
4. Students will be able to understand surface chemistry principles. Study properties and applications of superconductors. Apply surface characterization techniques.

### IC-29: Nuclear Chemistry

Introduction: The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy.

Nuclear structure: Shell model-salient features, forms of the nuclear potential, magic numbers, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.

Nuclear reactors :- General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors.

Nuclear reactions, fission and fusion, radio-analytical

Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect. Radio isotopes & its applications.

### IC-30: Zeolites and Molecular Sieves

**Introduction to porous materials:**

Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

**Zeolites:**

Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examplels of small, medium, large and extra large pore zeolites; general properties and application of molecular sieves.

**Characterization of zeolite:**

XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

### IC-31: Solid State Chemistry

Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.

Structure of ionic Crystals & Compounds: Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry $MX_2$, spinel structure, perovskite structure. AB [nickel arsenide (NiAs)], $AB_2$ [fluorite ($CaF_2$) and anti-fluorite structures, rutile ($TiO_2$) structure and layer structure [cadmium chloride and iodide ($CdCl_2$, $CdI_2$)].

**Crystal Defects and non-stoichiometry**:

Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in

silver halides; Calculation of number of defects and average energy required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.

**Preparative method of solids:**

Introduction, Ceramic method, microwave synthesis, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method, Chemical vapour Transport, Choosing a method for solids.

Crystal Growth: law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

### IC-32: Surface Chemistry & Superconductors

**Surface Chemistry:**

Mechanism of catalytic reactions on the surfaces – diffusion of reactants to the surfaces, adsorption of reactants, reaction within the adsorbed layer, desorption of the products, diffusion of the products away from the surface; The mechanism of chemisorption on metals – The formation of chemisorptions layer, the character and nature of the chemisorption bond, the mechanism of chemisorptions for some gases; Nature of adsorbates on surfaces.

**Superconductors:**

Discovery of super conductors, Meissner effect, Type I and II conductors, Leavitation, BCS theory and Cooper pairs, High Tc Super Conductors, applications of super conductors.

**SUGGESTED BOOKS**


1.Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.

2. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8and 9.

3.Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)

4.Breck.D.w. Zeolites molecular sieves- Structure, chemistry and use. John Wiley & Sons N.Y. (1974).

5.Solid-State Chemistry an Introduction ( 2nd Edition) – Lasley Smart and Elaine Moore ( Chapman & Hall 1996)

6. Solid State Chemistry- D.K.Chakraborty( New Age International Pvt.Ltd.New Delhi, 2000)

7. Introduction to Soilds-L.V.Azaroff( tata McGraw Hill Publication Ltd. New York)

8. Principles of the Solid State-H.V.Keer( Wiley Eastern Ltd.New Delhi, 1994)

9. Solid state Chemistry –N.B.Hannay( Prentice Hall, New Jersey, 1967)

10.Superconductivity, Joi, Khachan& Stephen Bio Science, -----

11.Chemisorption, B. M. W. Trapnell, Butterworths Scientific Publications, London, 1955.

12.Adsorption on solids, VladimirPonec, ZlatkoKnor, SlavojCerny, Butterworth & Co – publishers, 1974.

13.Catalysis: Principle and Applications, B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Narosa Publishing House, 2002.


## LABORATORY COURSES (III Semester)

## Paper CH (IC) 351: Synthesis and Characterization of Metal Complexes

Laboratory preparation and characterization of *3d* transition metal complexes of *tetrahedral*, *square planar* and *octahedral* geometries.

### Course Objectives

1. Synthesize 3d transition metal complexes with various geometries.
2. Characterize metal complexes using UV, IR, TGA, and other techniques.

3. Understand the principles and techniques for estimating metal content in complexes.
4. Explore solid phase synthesis and nanomaterial preparation.
5. Gain hands-on experience with advanced characterization methods like FT-IR and SEM.

## Learning Outcomes

1. Students will be able to successfully synthesize various 3d transition metal complexes.
2. Students will be able to characterize metal complexes using techniques such as UV, IR, TGA, and SEM.
3. Students will be able to estimate metal content and functional groups in complexes.
4. Students will be able to perform solid phase synthesis and nanomaterial preparation.
5. Students will be able to Interpret characterization data to understand complex structures and properties.

1. $VO(acac)_2$
2. $CoCl_2(Py)_2$
3. $Na[Cr(NH_3)_2(SCN)_4]$
4. Prussian Blue, Turnbull's Blue Complexes
5. $K_3[Cr(C_2O_4)_3]$ $3H_2O$ : UV, IR, TGA and estimation of oxalate.
6. Solid phase synthesis of trans-bis(glycinato)copper(II): IR, estimation of Cu by iodometry
7. $Fe(acac)_3$ : FTIR
8. Cis and trans $[CoCl_2(en)_2]Cl$ : conversion of cis to trans and trans to cis by IR.
9. Potassium bis(peroxo)oxo(1,10-phenanthroline)vanadium(V) trihydrate: IR,TGA, estimation of vanadium and peroxide
10. Tetra-butylammoniumhexamolybdate(VI): IR, estimation of Mo
11. $MnO_2$nano particles; SEM, SEM by adding CTAB

**SUGGESTED BOOKS**

1. *Practical Inorganic Chemistry*, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe,2ndedn John Wiley & Sons.
3. *Experimental Inorganic/Physical Chemistry*, M. A. Malati, Horwood Publishing,Chichester, UK (1999)

# Paper CH (IC) 352: Electro-analytical techniques

## Course Objectives

1. Perform potentiometric titrations. Calculate end point potentials for specific systems.
2. Determine $CO_3^{2-}$ and $HCO_3^-$ in mixtures by pH-metry. Determine dissociation constants of ethylenediamine, glycine, and histidine. Calculate binary constants for Cu (II)-en and Ni (II)-His systems. Determine stability constants of ternary systems.
3. Determine composition of Cu (II)-oxine and Cu (II)-EDTA complexes by conductometry. Study interactions of pyrophosphate with various cations. Determine aspirin content using KOH.
4. Estimate fluoride ion/nitrate ion/ammonia concentration in water by Ionimetry

5. Determine E½ of $Cd^{2+}$ and $Pb^{2+}$. Verify Ilkovic equation using $Cd^{2+}$ solution by polarography. Determine stability constants of $Cd^{2+}$ and $Pb^{2+}$ complexes.
6. Determine copper and nickel individually and in mixtures by electrogravimetry.

## Learning Outcomes

1. Students will be able to conduct accurate potentiometric titrations. Calculate end point potentials for specific titration systems.
2. Students will be able to determine carbonate and bicarbonate in mixtures by pH-metry. Calculate dissociation constants for ethylenediamine, glycine, and histidine. Evaluate binary constants for Cu(II)-en and Ni(II)-His systems. Determine stability constants for ternary systems.
3. Students will be able to Identify composition of Cu(II)-oxine and Cu(II)-EDTA complexes by conductometry. Analyze interactions of pyrophosphate with $Mg^{2+}$, $Ca^{2+}$, $Mn^{2+}$, and $Cu^{2+}$. Determine aspirin content using KOH.
4. Students will be able to estimate fluoride/nitrate/ammonia ion concentration in water by Ionimetry. Estimate nitrate ion concentration in water. Estimate ammonia concentration in water.
5. Students will be able to Determine E½ values for $Cd^{2+}$ and $Pb^{2+}$ by polarography. Verify the Ilkovic equation using $Cd^{2+}$ solution. Calculate stability constants for $Cd^{2+}$ and $Pb^{2+}$ complexes.
6. Students will be able to accurately determine copper and nickel, both individually and in mixtures by electrogravimetry.

**I Potentiometry**

Potentiometric Titrations and Calculation of End Point Potentials for the following systems:
i) $Fe^{2+}$and $VO^{2+}$ Mixture vs $Ce^{4+}$
ii) Assay of sulphanilamide
iii) Silver electrode for silver assay
iv) Mixture of halide anions using Silver electrode

**II pH-metry**

1. Determination of $CO_3^{2-}$ and $HCO_3^-$ in a mixture
2. Determination of the dissociation constants of
(i) Ethylenediamine (en)($H_2$ L) ( ii) Glycine (HL) (iii) Histidinemonohydrochloride ($H_2$L)
3. Determination of binary constants of i) Cu(II) -en and (ii) Ni(II) -His iii) Ni(II) – Gly Systems
4. Determination of stability constant of ternary (o-Phen-Ni(II)-His) system - Calculation of Log K.

**III Conductometry:**

1. Determination of the Composition of Cu(II)-oxine and Cu(II)-EDTA Complexes
2. Interaction of Pyrophosphate with $Mg^{2+}$, $Ca^{2+}$, $Mn^{2+}$ and $Cu^{2+}$
3. Determination of Aspirin with KOH

**IV Ion selective electrodes method (Ionimetry)**

1. Estimation of fluoride ion in water
2. Estimation of nitrate ion in water
3. Estimation of ammonia in water

**V Polarography**

1. Determination of $E_{½}$ of $Cd^{2+}$ and $Pb^{2+}$

2. Verification of Ilkovic equation by using $Cd^{2+}$ solution
3. Determination of Stability Constants of $Cd^{2+}$ and $Pb^{2+}$ complexes

**VI Electrogravimetry**

1. Determination of Copper and Nickel individually and in a Mixture

**SUGGESTED BOOKS**


1. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition Elbs Publication 1969.
2. Vogel's Text Book Of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications 1988.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
4. Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC 1988.
5. Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York – 1996.
6. Analytical Chemistry by Gary D.Christian 6th EditionJohnWiley&Sons Inc New York 1994.


# M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
# SEMESTER-IV
# PAPER I

## CH(IC)401T: Molecular Spectroscopy of Inorganic Compounds

**IC-33: Multinuclear NMR**
**IC-34: Advanced NMR techniques**
**IC-35:Applications of ESR to Metal Complexes**
**IC-36:Mossbauer Spectroscopy and Nuclear Quadrupole Resonance Spectroscopy**

## Course Objectives

1. Understand principles of multinuclear NMR. Study NMR techniques for various nuclei. Apply multinuclear NMR to structural analysis.
2. Learn advanced NMR techniques. Understand 2D NMR methods. Apply advanced NMR for detailed molecular characterization.

3. Understand principles of Electron Spin Resonance (ESR). Study ESR applications in metal complexes. Analyze electronic structure and bonding in metal complexes using ESR.
4. Understand Mossbauer spectroscopy principles. Learn Nuclear Quadrupole Resonance (NQR) spectroscopy. Apply these techniques to study material properties and structures.

## Learning Outcomes

1. Students will be able to understand principles of multinuclear NMR. Use NMR techniques for different nuclei. Analyze structures using multinuclear NMR.
2. Students will be able to comprehend advanced NMR methods. Apply 2D NMR techniques. Characterize molecules in detail using advanced NMR.
3. Students will be able to understand ESR principles. Apply ESR to study metal complexes. Analyze electronic structure and bonding in metal complexes.
4. Students will be able to understand Mossbauer spectroscopy principles. Learn NQR spectroscopy techniques. Apply these methods to study material properties and structures.

### IC-33: Multinuclear NMR

$^{13}C$ nmr spectroscopy: CW and PFT techniques. Types of $^{13}C$ nmr spectra: undecoupled, proton-decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. $^{13}C$ chemical shifts, factors affecting the chemical shifts.

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes $[Pd\{P(CH_3)_3\}_2I_2]$. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity ($PF_5$, $[Rh(PR_3)_5]^+$, $[Fe\{Cp\}_2(CO)_2]$ ) -ΔR, the Ring Contribution to $^{31}P$ Chemical Shifts –Metal and Chelate size on ΔR. Applications of $^1H$, $^{13}C$, $^{19}F$, $^{31}P$ and $^{15}N$ to simple inorganic and Coordination Compounds - 1)$^1H$-NMR: $PtHCl(PEt_3)_2$,$Pt(NH_3)_3(CH_3)_3$, $BH_4^-$, $NH_4^+$, $CH_3CN$, [$^6$h- $C_7H_8$ $Mo(CO)_3$], [$^7$h-$C_7H_7Mo(CO)_3]^+$, $B_2H_6$; $^{29}SiH_3SiH_3$, 2)$^{19}F$: $BF_4^-$, $H_2PF_3$ 3)$^{31}P$: $Mo(CO)_3(PPh_3)_3$, [Rh $(PPh_3)_3Cl$] ,trans-$[PtCl_4(PEt_3)_2]$ , $^{31}PF_2H(^{15}NH_2)_2$ 4) 13C; [$^4$h $C_8H_8Ru(CO)_3$], $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$, FeICp$(CO)_{12}$, [$^{13}C^{15}N$ $Co(DH)_2$Pyridine]. $^{13}C\{^1H\}$ NMR spectrum of σ-bonded $C_6H_5$ ligand.

### IC-34: Advanced NMR techniques

Spin-Lattice ($T_1$) and Spin-Spin Relaxation ($T_2$). Spin Echo Polarization Transfer – Spin Echo Measurements. $^{13}C$-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY( Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

### IC-35:Applications of ESR to Metal Complexes

Principle- Selection Rules – Instrumentation- Microwavesource (energy bands). Application of ESR to the study of simple free radicals: methyl ($CH_3^{\cdot}$), amine ($NH_2\cdot$), diphenylpicrylhydrazyl,cyclopentadienyl ($C_5H_5^{\cdot}$), hydroxy methyl ($CH_2OH\cdot$) radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of $d^1$-$d^9$ Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of

g values with simple examples. Intensities of 'g∥ and g⊥peaks. Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine. $[(NH_3)_5\ Co\ O_2\ Co\ (NH_3)_5]^{5+}$, Cu(II)- diethyldithiophosphinate, Vanadyldithiophsphinate, Copper(II) tetraphenylporphyrin, Co(II)- phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) $MnF_6^{4-}$, ii) $CoF_6^{4-}$, and $CrF_6^{3-}$. ESR spectra of dinuclear Cu (II) complexes.

**IC-36 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy**

**Mossbauer Spectroscopy:** Principle, Experimental Considerations and Presentation of the Spectrum - Isomer Shifts – Quadrupole splitting and Magnetic hyperfine splitting - Selection Rules.

**Applications**

**Iron Compounds:** Low-spin and High-spin Fe(II) and Fe(III) Complexes - π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins.

**Tin Compounds:** Tin Halides and Organotin Compounds.

**Iodine Compounds:** Isomer Shifts of $^{127}I$ and $^{129}I$ - Applications to Alkali metal iodides and Molecular Iodine. Mossbauer spectra of $IF_6^-$ and $IF_6^+$

**Nuclear Quadrupole Resonance Spectroscopy:** Principle, nuclear quadrupole resonance experiment, Structural information from NQR spectra- $PFCl_4$, $PCl_4Ph$, $Ga_2Cl_7^-$ and $TeCl_4$ Interpretation of nuclear quadrupole coupling constants.

**SUGGESTED BOOKS**


1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and
2. S. Craddock, ELBS.
3. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
5. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing, 1992.
6. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, 1976.
7. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, 1971.
8. Principles of Instrumental Analysis, Skoog, Holler and Nieman.
9. Instrumental Techniques for Analytical Chemistry, Frank Settle.
10. Principles of Analytical Chemistry, M. Valcarcel.
11. Physical Methods in Advanced Inorganic Chemistry, Hill and Day
12. Magneto Chemistry, Dutta &Shyamal Oxford Chemistry Primers, Vol 62


# PAPER II

## CH(IC) 402T: Bioinorganic Chemistry

**IC-37: Metal ions Interactions with Nucleic acids and their constituents**
**IC-38: Transport of Electrons and Metal ions**
**IC-39: Metallo-Enzymes of Iron, Zinc and Nickel**
**IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenumand Manganese**

### Course Objectives

1. Understand interactions between metal ions and nucleic acids. Study binding mechanisms and effects on nucleic acids. Explore biological and therapeutic implications.

2. Learn mechanisms of electron and metal ion transport. Study biological transport systems. Analyze the role of metal ions in cellular processes.
3. Understand the function of iron, zinc, and nickel metallo-enzymes. Study the catalytic mechanisms of these enzymes. Explore their biological significance and applications.
4. Learn about cobalt, copper, molybdenum, and manganese metallo-enzymes. Understand the catalytic processes and mechanisms. Study their roles in biological systems and applications.

## Learning Outcomes

1. Students will be able to understand metal ion interactions with nucleic acids. Analyze binding mechanisms and effects. Recognize biological and therapeutic implications.
2. Students will be able to understand electron and metal ion transport mechanisms. Study biological transport systems. Analyze the role of metal ions in cellular processes.
3. Students will be able to understand the function of iron, zinc, and nickel metallo-enzymes. Study catalytic mechanisms of these enzymes. Explore their biological significance and applications.
4. Students will be able to understand the role of cobalt, copper, molybdenum, and manganese metallo-enzymes. Study catalytic mechanisms and processes. Analyze their roles in biological systems and applications.

### IC-37: Metal ions Interactions with Nucleic acids and their constituents

Nucleic Bases, Nucleosides and Nucleotides. Proton Binding Sites of Nucleic Acid Constituents-Purine and Pyrimidine Bases, Nucleosides and Nucleotides. The covalent structure of polynucleotides, secondary structure of DNA: The double helix anti and syn conformations of nucleotides. B, A, & Z forms of DNA. General Factors that influence Metal Ion Binding Sites in Solution – Specific Metal Ion Binding to Nucleic Bases, Nucleotides and Nucleosides in Solution: Stability of Phosphate- Metal ion complexes, Metal binding Metal Ion Complexes, Metal Binding Sites in Nucleosides, Nucleotide - Metal Ion Interactions - Intramolecular Equilibrium Constant KI, Percentage of Closed Isomers - Outer Sphere and Inner Sphere Isomers of M-ATP Complexes and Metal Ion Nucleic Base Interactions.
*Metal-DNA and RNA Interactions*: Potential Binding Sites (Elementary Treatment) – Influence of Metal Ions on Stability of Nucleic Acids.

### IC-38: Transport of Electrons and Metal ions

*Transport of Electrons*: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe,3Fe, 4Fe, 8Fe Proteins) -High Potential Iron-Sulphur Proteins – Structural andSpectral features of Iron-Sulphur Proteins - Electron-transport by Cytochromes,Azurin and Plastocyanin - Importance of Structures of Azurin and Plastocyanin infacilitating Rapid Electron Transport, acotinase- Fe-S enzyme.
*Transport and Storage of Metal Ions*: Iron-Transport by Transferrin and Siderophores – Ferritin in Iron Storage - Transport of Na+ and K+ across Cell Membranes by $Na^+$- $K^+$ ATPase - Transport of Calcium across Sarcoplasmic Reticulam by $Ca^{2+}$-ATPase.

### IC-39: Metallo-Enzymes of Iron, Zinc and Nickel

**Iron Enzymes:** Structural and Mechanistic Aspects of Cytochrome P450, Cytochrome oxidase,Catalase and Peroxidase - Role of the Metal Ion.
**Zinc Enzymes:** Structural and Mechanistic Aspects of Carbonic Anhydrase, Carboxy Peptidase,Leucin – aminopeptidase, Thermolysin, Alcohol Dehydrogenase - Role of Zinc.
**Nickel Enzymes:** Urease, Hydrogenase and Factor F430: Reactions Catalyzed, MechanisticAspects.

**IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese**

**Cobalt Enzymes:** Cobalt in Vitamin B12 - Structural Features of Vitamin B12 with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B12 and Active Enzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii)DeoxyadenosylCobalamin - Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B12.

**Copper Enzymes:** Types of Copper in Biological Systems - Structural and Mechanistic Aspects of Superoxide Dismutase, Laccase and Galactose oxidase.

**Molybdenum Enzymes:** Biological Roles and Mechanistic Aspects of Nitrogenase, Xanthineoxidase and Sulfite oxidase.

**Manganese Enzymes*:*** Arginase, Water – oxidase.

**SUGGESTED BOOKS**


1. Biochemistry - Geoffrey L. Zubay.
2. Biochemistry - Mary K. Campbell. (added these books)
3. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University ScienceBooks, California USA 1994.
4. Principles of Bioinorganic Chemistry, S.J. Lippard and M.Berg University ScienceBooks, California 1994.
5. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams OxfordUniversity Press 1991.
6. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York
7. Inorganic Biochemistry, J.A. Cowan, VCH publishers 1993.
8. Advances in Inorganic Biochemistry, edited by G.L.Eichorn&Marzilli
9. Bioinorganic Chemistry, Vol-I edited by G.L.Eichorn.
10. Interactions of metal ions with nucleotides and nucleic acids and their constituents Helmut Sigel Chem. Soc. Rev., 1993,22, 255-267.


# PAPER III

## CH(IC)403T( Elective IIIa ):Medicinal Inorganic Chemistry, Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials

**IC-41: Metal complexes in Clinical Chemistry**
**IC-42: Metal complexes as Drugs and Anticancer agents**
**IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA**
**IC-44: Applications of Nanomaterials**

### Course Objectives

1. Understand the role of metal complexes in clinical diagnostics. Study the therapeutic applications of metal complexes. Explore the use of metal complexes in medical imaging and treatment.

2. Learn about metal complexes used as drugs. Understand the mechanisms of metal-based anticancer agents. Explore the development and applications of these drugs.
3. Understand spectroscopic techniques for analyzing drug/metal-DNA interactions. Study the binding mechanisms of drug/metal complexes to DNA. Explore applications in drug design and development.
4. Understand the properties of nanomaterials. Learn about the synthesis and characterization of nanomaterials. Explore various applications in electronics, medicine, and materials science.

## Learning Outcomes

1. Students will be able to understand the role of metal complexes in clinical diagnostics. Study therapeutic applications of metal complexes. Explore their use in medical imaging and treatment.
2. Students will be able to understand metal complexes as pharmaceutical agents. Analyze mechanisms of metal-based anticancer drugs. Explore development and applications of these drugs.
3. Understand spectroscopic techniques for drug/metal-DNA interactions. Analyze binding mechanisms of drug/metal complexes to DNA. Apply knowledge in drug design and development.
4. Understand the properties of nanomaterials. Learn synthesis and characterization techniques. Explore applications in electronics, medicine, and materials science.

**IC-41: Metal complexes in Clinical Chemistry**

Theory and mode of action of therapeutic chelating agents , Single ligand Chelation Therapy – Aminopolycarboxylic acids, Desferrioxamine, pencillamine, triethylenetetramine, Mixed ligand chelation therapy - Metallothionens in detoxification. Role of metal ions in the action of antibiotics: Bleomycin, adriamyacin and tetracyclines. Gold-Containing drugs used in therapy of Rheumatoid arthritis - A therapeutic agent for Menkes disease: Copper-histidine - Anti viral chemotherapy and metal peptide interaction.

**IC-42: Metal complexes as Drugs and Anticancer agents**

**Introduction to Pt(II) chemistry**– Thermodynamic and kinetic principles – *Cis*and *Trans* influences – Thermodynamic and kinetic aspects. Steric and electronic tuning of reactivity.

**Platinum complexes in cancer therapy:** Discovery applications and structure-effect Relationships. Cis-platin(cis$Pt(NH_3)_2Cl_2$) mode of action. Potential binding sites on nucleic acids and their bases and proteins. Drug resistance and DNA repair mechanism.

**Physical effects of metal complex:** DNA binding, unwinding, shortening and bending of the double helix. Biological consequences of platinum –DNA binding. Organic intercalators asdonor – acceptor pairs; Transition metal complexes as donor acceptor pairs. Non classical platinum antitumour agents.

**IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA**

Introduction to DNA binding studies. Cooperativityanticooperativity, the excluded site model. UV-Vis Absorption Spectroscopy and ligand/drug/metal complex DNA binding studies. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies. Fluorescence titrations and binding constants. Salt back titrations interpretation of the data, the binding analysis,obtaining equilibrium binding isotherms. Dependence of $K_{obs}$on salt concentration, cation effects on ligand nucleic acid equilibria, Competitive effects of monovalent and divalent cations for binding.

Record's polyelectrolyte theory and its importance. Equilibrium dialysis. Partition analysis, competitive equilibrium dialysis to assess B & Z DNA binding. Competition dialysis to assess base and sequence specificity, viscosity studies. Tertiary structure of DNA, Supercoiled DNA(Form-I), Nicked DNA (Form-II) and Linear DNA(Form-III). DNA cleavage activity with ligand/metal complexes-Analysis by Gel electrophoresis.

**IC-44: Applications of Nanomaterials**

Nanotechnology in modern technology in relation to electronic, biological, consumer and domestic applications. Energy related application: photo-volatile cells. Energy storage nanomaterials.
Sensors: Agriculture, health and medical, food, security.
Applied nanobiotechnology and nanobiomedical science drug delivery, drug targeting, biosensors, bioimaging, neutron capture therapy.

**SUGGESTED BOOKS**


1. Bioinorganic Chemistry. Inorganic elements in the Chemistry of life, WolfgangKaim&BrigetteSchwederdki.
2. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University ScienceBooks, California USA 1994.
3. Handbook of Metal-Ligand interactions in Biological fluid Bioinorganic medicine, Vol – Edt. Guy Berthon.
4. Bioinorganic Chemistry, Rosette M. RoatMalone.
5. Photoreactions of Metal complexes with DNA, A. Krisch – De Mesmacker et al.
6. Drug - Nucleic Acid Interactions, Volume 340 Jonathan B. Chaires, Michael J. WaringAcademicPress,2001.
7. Mechanistic Bioinorganic Chemistry Edited by byH.Holden Thorp and Vincent L. Pecoraro, Chemical Society, Washington DC 1995.
8. Metal Complex -DNA Interactions, Editor(s): Nick Hadjiliadis, EinarSletten, Copyright @ Blackwell Publishing Ltd.
9. Gel Electrophoresis - Principles and basics edited by SamehMagdeldin ISBN 978 - 958 -51-0458-2, 376 pages, Publisher: InTech, April 04, 2012
10. Encylopedia of nanomaterials and nanotechnologies, H. S. Nalva.
11. Nanostructures materials: Processing, Properties and applications, C. C. Kouch, WilliamAndrew publications, New york, 2002.
12. Introduction to nanotechnology, C. P. Poole Jr, F. J. Owens, 2nd edition, Wiley-India,Delhi, 2008.


# PAPER III

## CH(IC)403T( Elective IIIb ):Analytical Techniques -III

**IC-45: Electroanalytical Methods**
**IC-46: Radiochemical Methods**
**IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry**
**IC-48: Industrial Analysis**

**IC-45: Electroanalytical Methods**

## Course Objectives

1. Understand principles of electroanalytical techniques. Learn methodologies such as voltammetry and coulometry. Apply electroanalytical methods for chemical analysis.
2. Understand principles of radiochemical techniques. Learn about radioactive decay and detection methods. Apply radiochemical methods in chemical analysis and research.
3. Understand principles of fluorescence, phosphorescence, nephelometry, and turbidimetry. Learn the instrumentation and methodologies for each technique. Apply these methods for qualitative and quantitative analysis.
4. Understand principles of industrial chemical analysis. Learn techniques used in quality control and process monitoring. Apply analytical methods in various industrial sectors.

## Learning Outcomes

1. Students will be able to understand electroanalytical techniques. Use voltammetry and coulometry for analysis. Apply electroanalytical methods in chemical analysis.
2. Students will be able to understand radiochemical techniques. Use radioactive decay and detection methods. Apply radiochemical methods in research and analysis.
3. Students will be able to understand fluorescence, phosphorescence, nephelometry, and turbidimetry principles. Use instrumentation and methodologies for each technique. Apply these methods for qualitative and quantitative analysis.
4. Students will be able to understand industrial chemical analysis principles. Use techniques for quality control and process monitoring. Apply analytical methods in various industrial sectors.

**pH-metry:** Accuracy of direct potentiometer measurements. The Glass pH electrode – Theory, construction, standard buffers, accuracy of pH measurements, measurements with the pH – meter, pH titration of unknown soda ash.

**Electrogravimetry:** Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current. Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

**Coulometry :** Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.

**High Frequency Titrations:** Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages.

### IC-46: Radiochemical Methods

Radioactive nucleotides, Instrumentation – measurement of alpha, Beta particles and Gamma radiation. Radio tracers and tracer techniques, applications of Tracer techniques,

Neutron activation analysis: Neutron sources, interaction of neutrons with matter. Theory of activation methods, Experimental considerations, Nondestructive and destructive methods, applications.

Isotopic dilution analysis: Principles, theory and Applications.

Radiometric titrations: Principle, Procedure, advantages & disadvantages, applications to various types of titrations, problems based on the techniques.

Applications of Radio Chemical Methods in Biology, Agriculture and Environment

## IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry

**Fluorimetry and Phosphorimetry**: Theory of Fluorescence and Phosphorescence- Excited states producing Fluorescence and Phosphorescence. Rates of absorption and emission. Deactivation processes, Variables affecting Fluorescence and Phosphorescence. Types of Photoluminescence spectra for Phenanthrene. Instrumentation – Components of Fluorimeter, Spectroflourimeters and Phosphorimeters. Applications of Fluorimetry - Determination of Inorganic Cations, Fluorimetric reagents. Fluorimetric determination of organic species – Thiamine, Aneurine Hydrochloride, Polycyclic aromatic hydrocarbons. Phosphorimetry- Determination of Aspirin in blood serum. Chemiluminescence- Origin, measurements. Analytical applications- Atmospheric pollutants (Oxides of Nitrogen and Sulphur compounds, Ozone).

**Nephelometry and Turbidimetry**: Light scattering, principle and theory ofNephelometry and Turbidimetry, Effect of concentration, particle size and wavelength on scattering, instrumentation for Nephelometry and Turbidimetry. Turbidimetric titrations. Applications of Nephelometry and Turbidimetry.

## IC- 48: Industrial Analysis

**Analysis of Ferroalloys:** Analysis of steel - Molybdenum, Phosphorous.

**Analysis of non- Ferrous alloys**: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder.

**Analysis of Cement**: Composition of Portland cement, estimation of Aluminium oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography.

**Analysis of Oils & Fats:** Theory, Melting point of fats, Chemical Characteristics: Saponification value, Iodine value, Thiocyanogen value, ketone or perfume rancidity.

**Soaps & Detergents:** Composition of Soaps. Determination of low level Surfactants, determination of Germicides in soaps and detergents by photometric method, analysis of phosphates by paper chromatography, determination of detergent alkylates by Mass Spectrometry.

**Paints& Pigments**: Constituents of Paints, Analysis of $TiO_2$ in Titanium dioxide pigments by XRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis of polyesters, acrylics by Gel permeation chromatography.

**SUGGESTED BOOKS**


1. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed.Blackwell Science, 2000
2. Principles of Instrumental Analysis: Holler, Skoog and Crouch, 6th education, Cengage Learning 2007.
3. Instrumental methods of chemical analysis B.K. Sharma, Goel Publishing House.
4. Analytical Chemistry: Gary D Christian.6th edition.
5. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
6. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork, 2003.
8. Analytical Chemistry an Introduction, Crouch, 7th Ed. Saunders College Publishing,2000.
9. Standard methods of Chemical analysis, 6th ed., volumes I to IV. Edited by F.J. Welcher: D. Von NostrnadCo. Inc., Princeton N.J. 1966.
10. Biochemical Methods – S. Sadasivam, A. Manickam, 2nd ed., New Age International (P) Ltd., 1997.


# PAPER IV

## CH(ID) 404T( Elective IVa ): Interdisciplinary Course (ID) (Environmental and Applied Analysis)

**IC-49: Clinical and Pharmaceutical Analysis**
**IC-50: Food and Agricultural analysis**
**IC-51: Analysis of Air and Water Pollutants**
**IC-52: Drinking Water and Sewage Water Treatment**

## Course Objectives

1. Understand principles of clinical and pharmaceutical analysis. Learn techniques for drug and metabolite analysis. Apply analytical methods in clinical diagnostics and pharmaceutical quality control.
2. Understand principles of food and agricultural analysis. Learn techniques for detecting contaminants and nutrients. Apply methods to ensure food safety and quality.
3. Understand principles of pollutant analysis in air and water. Learn techniques for detecting and quantifying pollutants. Apply methods for environmental monitoring and compliance.
4. Understand principles of water treatment processes. Learn techniques for treating drinking and sewage water. Apply methods to ensure water quality and safety.

## Learning Outcomes

1. Students will be able to understand principles of clinical and pharmaceutical analysis. Apply analytical techniques in drug analysis and quality control. Analyze biological samples for diagnostic purposes.
2. Students will be able to understand principles of food and agricultural analysis. Apply techniques to assess food quality and safety. Analyze agricultural products for contaminants and nutrients.
3. Students will be able to understand principles of pollutant analysis in air and water. Apply techniques for monitoring and quantifying pollutants. Assess environmental impact and compliance with regulations.
4. Students will be able to Understand principles of water treatment for drinking and sewage water. Apply techniques to ensure water quality and safety. Evaluate effectiveness of treatment processes in removing contaminants.

**IC-49: Clinical and Pharmaceutical Analysis**

**Clinical analysis**: Analysis of Carbohydrates and their significances – Fasting, random and post pandrial glucose tests, Estimation of Glucose in serum. Analysis of lipids and their significances –Test for cholesterol. Analysis of proteins and their significance – Estimation of total protein in serum.
Analysis of Major metabolites and their significance – Determination of Blood urea and Creatinine in urine. Analysis of ions and their significance: Estimation of Na, K, Ca, bicarbonates and phosphate in serum. Analysis of Hormones and their significance-ELISA and RIA.

**Pharmaceutical analysis**: Determination of Diclofenac (non-aqueous titration), Calcium inVitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry),Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin,paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid indipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC).Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

## IC-50: Food and Agricultural analysis

**Analysis of Chemical additives**: Division of colour additives (Coal-tar dyes, vegetable colours and mineral colours). **Chemical preservatives** and synthetic sweetening agents (organic-ether extractable and non-ether extractable) $SO_2$, Sodium Benzoate, Sorbic acid, Benzoic acid.

**Antioxidants**: Types of Antioxidants used in foods, Analysis of Butylatedhydroxy toluene (BHT), propyl – gallates (PG), Octylgallates (GO), dodecyl gallates (DG) by TLC & GC.

**Food adulteration**: Common adulterants in food, contamination of food stuffs. Microscopic examinations for food adulterants.

**Analysis of Soil** – Determination of pH, conductivity, cation exchange capacity, total organic matter, nitrogen, phosphorous, potassium, S, Ca, Mg, Ca+Mg, Zn, Cu, Fe, Mn, B, Mo, Cd, Cr, Ni, Pb.

**Analysis of Fertilizers** – Moisture determination by Karl Fischer titration methods. Determination of Ammonical nitrogen and Ammonical nitrate nitrogen. Determination of total phosphates as $P_2O_5$. Estimation of potassium, Estimation of micronutrients by AAS.

**Analysis of Pesticides**: Analysis of Organo-chlorine pesticides (Cypermethrin) by Gas Chromatography. Determination of Malathion, Methyl parathion and DDT residues in vegetables and food grains.

## IC-51: Analysis of Air and Water Pollutants

Air quality standards, sampling, analysis of air pollutants-$SO_2$ (UV-Vis, IR), $H_2S$ (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & $CO_2$ (IR, AAS & GC), Hydrocarbons ( GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, $O_3$ (Chemiluminiscence& Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – $CN^-$, $Cl^-$, $F^-$, $NO_2^-$, $NO_3^-$ (spectrophotometry), $SO_4$, $PO_4$. Determination of BOD, COD, TOC & DO. Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

## IC-52: Drinking Water and Sewage Water Treatment

**Hardness:** causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, Alkalinity of water and its estimation.

**Treatment of Water for Municipal Supply:** Characteristics of potable water/Domestic water, WHO standards, and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Physical Methods-Boiling, Exposure to Sunlight, Disinfection with UV light, Chemical Methods – Ozonization, Chlorination, Breakpoint chlorination and Dechlorination

**Desalination of Brackish Water:**Treating saline water: distillation, electrodialysis, reverse osmosis (RO).

**Mineral Water and Purified Water:** Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process, Purified Water-Purification methods-Distillation, Double distillation, Deionization - Co-current deionization, Counter-current deionization, Mixed bed deionization, Demineralization, Uses of purified water- Laboratory use, Industrial uses and other uses; Health effects of drinking purified water

**Sewage Water Treatment:** Domestic sewage - Physical, Chemical, and Biological Characteristics of Domestic Sewage, Municipal sewage, Sewage Composition and Contaminants, Sewage Treatment - On-Site Sewage Treatment Systems and Off-Site Sewage Treatment Systems

**SUGGESTED BOOKS**


1. Medical Laboratory Technology – Mukherjee,McGraw Hills,1988.
2. Medical Laboratory Technology – RamnikSood, Medical Publishers Pvt. Ltd., 1999.
3. Biochemical Methods – S. Sadasivam, A. Manickam, 2nd ed., New Age International (P) Ltd., 1997.
4. Practical Pharmaceutical Chemistry, A.H. Beckett et al, 3rd ed. – Vol. 1 & Vol. 2 CBS Publishers & Distributors, 1986.
5. Pharmaceutical Analysis - P. Primoo. CBS Publishers, New Delhi, 1999.

6. Text book of Pharmaceutical Analysis – Kenneth. A. Connors, John Wiley & Sons, 1999.
7. Pharmaceutical Chemistry, Instrumental techniques vol-2, Ed. Lesile. G.Chatten.
8. Pharmaceutical Drug Analysis – Asuthoshkar, Minerva Press, 2001.
9. Handbook of analysis and quality control for fruit and vegetables products – S. Ranganna, 2nd edition, Tata McGraw-Hill Publishing Ltd., 1986
10. Introduction to the Chemical Analysis of Foods, S. Suzanne Neilsen, CBSPublishers, New Delhi, 2002.
11. A Text book of Soil Chemical Analysis – P.R. Hesse, CBS Publications, 1998.
12. Methods of Analysis of Soils, Plants, Water and Fertilizers – Ed, HLS Tandon, FDCO publications, New Delhi, 1999.
13. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd.
14. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995.
15. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie AcademiProfessional.
16. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
17. "A Textbook of Engineering Chemistry", Dr. Y. BharathiKumari and Dr. JyotsnaCherukuri, VGS Publications, First Edison, India, 2009.
18. "Engineering Chemistry", Jain P C and Monica Jain, 15th Edition, DhanpatRai Publishing Company Ltd, New Delhi, India, 2005.
19. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India
20. Water Encyclopedia - Domestic, Municipal, andIndustrialWaterSupply and Waste Disposal, Jay H. Lehr and Jack Keeley, Wiley-Interscience, Published by John Wiley & Sons, Inc., Hoboken, New Jersey.
21. Handbook of Water and Wastewater Treatment Technologies, Nicholas P. Cheremisinoff, PublishedbyButterworth-Heinemann, 225Wildwood Avenue, Woburn, MA 01801-2041
22. Purified water: https://en.wikipedia.org/wiki/Purified_water#Purification_methods

# PAPER IV

## CH(ID) 404T( Elective IVb ): Interdisciplinary Course (ID) (Inorganic Material Chemistry)

**IC-49: Composite Materials**
**IC-50: Liquid Crystals**
**IC-51: Explosives and Propellants**
**IC-52: Fuels and Combustion**

## Course Objectives

1. Understand principles of composite materials. Learn about types and properties of composites. Explore applications in various industries.
2. Understand principles of liquid crystals. Learn about phases and properties of liquid crystals. Explore applications in display technology and other fields.
3. Understand principles of explosives and propellants. Learn about synthesis and properties of energetic materials. Explore applications in defense and industrial sectors.
4. Understand principles of fuels and combustion. Learn about types of fuels and combustion processes. Explore efficiency and environmental impact of combustion technologies.

## Learning Outcomes

1. Students will be able to understand the principles and types of composite materials. Analyze properties and applications of composites in various industries. Evaluate advancements and future trends in composite technology.
2. Students will be able to understand the phases and properties of liquid crystals. Apply knowledge to technological applications in displays and optics. Analyze recent developments and emerging uses of liquid crystals.
3. Understand the chemistry and properties of explosives and propellants. Evaluate safety, efficiency, and environmental impact of energetic materials. Apply knowledge to defense, mining, and aerospace industries.
4. Understand the types of fuels and combustion processes. Analyze efficiency, emissions, and environmental impact of combustion technologies. Apply principles to optimize fuel use and develop sustainable combustion solutions.

### IC-49: Composite Materials

Introduction, Advantageous Properties of the Composites, Constituents of Composites, Types of Composites – Fibre-reinforced composites (Glass, carbon, Armid, Alumina reinforced composites), Particulate composites, Layered composites, Processing of Fibre-reinforced Composites, Micromechanics of Fibre and Particle Reinforced Composites, Fabrication of the Composites.

**Refractories:** Characteristics and Classification of Refractories, Properties of Refractories, Manufacture of Refractories, Common Refractories Bricks – Silica Bricks, Alumina Bricks, Magnesite Bricks, Dolomite Bricks, Carbon Bricks and Chromite Bricks.

**Ceramics:** Plasticity of Clays, Whitewares or White-Pottery, Manufacture of White-Pottery, Glazing, Methods of glazing, Earthenwares and Stonewares.

### IC-50: Liquid Crystals

Introduction, Types of Mesophases, Characterization of Liquid Crystals, Physical Properties of Liquid Crystals, Structure of Liquid Crystal forming compounds, Classification of Liquid Crystals-Thermotropic Liquid Crystals and Lyotropic Liquid Crystals, Chemical Properties of Liquid Crystals, Applications with special reference to Display systems, Applications and Importance of Lyotropic Liquid Crystals, Future of Liquid Crystals.

### IC-51: Explosives and Propellants

**Explosives**: Introduction, Classification of Explosives, Primary Explosives, Low Explosives, High Explosives, Precautions During Storage of Explosives, Blasting Fuses, Manufacture of Important Explosives-Lead azide, Diazonitrophenol (DDNP), Trinitrotoluene (TNT), Nitroglycerine (NG) or Glycerol trinitrate (GTN), Pentaerythritaltetranitrate (PETN) and RDX; Recent uses of Explosives

**Propellants:** Rocket Propellants - Introduction, Principle of Rocket Propulsion, Classifications of Propellants-Solid propellants, Composite propellants, Liquid Propellants, Mono-propellants, Bi-propellants; Differences between Solid propellants and Liquid Propellants

### IC-52: Fuels and Combustion

Introduction, Classification of Fuels, Calorific Value, Characteristics of a Good Fuel, Theoretical Calculation of Calorific value of a Fuel, Coal, Classification of Coal by Rank, Analysis of Coal – Proximate analysis and Ultimate analysis, Metallurgical Coke, Types of Carbonization of Coal – Low-temperature and high temperature carbonization, Manufacture of Metallurgical Coke by Beehive oven process, Petroleum, classification of petroleum, Refining of crude oil, Cracking – Thermal cracking, Catalytic cracking- Moving-bed catalytic cracking, LPG as a Fuel, Natural Gas, Producer Gas, Water Gas (or Blue Gas), Non-Conventional Sources of Energy-Solar energy, Solar cells and Uses of solar cells.

**Combustion:**Combustion, Mass Analysis from Volume Analysis and Vice Versa, Analysis of Flue Gas

**SUGGESTED BOOKS**

1. "Liquid Crystals, Nature's delicate phase of matter", Peter J Collings, Princeton University Press, 2002
2. "Liquid Crystals: Fundamentals", Shri Singh, World Scientific Publishing Company; 1st edition (November 7, 2002)
3. "Science of Engineering Materials", C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
4. "Engineering Chemistry", Jain P C and Monica Jain, 15th Edition, DhanpatRai Publishing Company Ltd, New Delhi, India, 2005.
5. A Text book of Engineering Chemistry", Shashi Chawla" DhanpatRai Publishing Company (P) Ltd., New Delhi, India, 2007.
6. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India.
7. "A Textbook of Engineering Chemistry", Dr. Y. BharathiKumari and Dr. JyotsnaCherukuri, VGS Publications, First Edison, India, 2009

## Paper CH (IC) 451: Conventional Methods of Analysis

### Course Objectives

1. Determine $Ca^{2+}$, $Mg^{2+}$, $CO_3^{2-}$, $HCO^{3-}$ in soil samples by Titrimetry. Analyze saponification value, iodine number, acid value, and ester value of oil samples. Quantify ascorbic acid in Vitamin C tablets using iodometry.
2. Measure dissolved oxygen content in water samples. Determine Chemical Oxygen Demand (COD) in water samples. Quantify residual chlorine using iodometry in water samples. Determine fluoride concentration using the Zirconium Alizarin method in water samples. Measure sulfate concentration using spectrophotometry, turbidimetry, or nephelometry in water samples.
3. Separate $Fe^{3+}$ and $Ni^{2+}$ using tri-n-butylphosphite (TBP) via solvent extraction. Identify cations (Co (II), Ni (II), Cu (II)) using paper chromatography. Separate Fe (III) and Al (III) using column chromatography. Separate $Fe^{3+}$ and $Ni^{2+}$ using strongly basic anion resin.

### Learning Outcomes

1. Students will be able to Develop skills in quantitative analysis of soil components. Master techniques for assessing oil quality parameters. Apply iodometric methods for analyzing ascorbic acid in Vitamin C tablets.
2. Understand and apply methods for assessing water quality parameters like dissolved oxygen and COD. Gain proficiency in determining residual chlorine and fluoride concentrations in water. Learn techniques for measuring sulfate levels in water using spectrophotometry, turbidimetry, or nephelometry.
3. Acquire proficiency in separating metal ions using solvent extraction and chromatographic techniques. Develop skills in identifying cations using paper

chromatography. Master techniques for separating and analyzing metal ions using ion exchange resins and chromatography.

**I. Titrimetry:**

1. Determination of $Ca^{2+}$, $Mg^{2+}$, $CO_3^{2-}$, $HCO_3^-$ in soil sample
2. Determination of saponification value, Iodine number, acid value and ester value of an oil sample (5-6 samples and comparative study)
3. Determination of Ascorbic acid in Vit.C tablet by iodometry (2-3 samples)

**II Water analysis**:

1. Determination of Dissolved Oxygen
2. Determination of COD
3. Determination of residual Chlorine in water by Iodometry
4. Determination of Fluoride by Zirconium Alizarin Method
5. Determination of Sulphate by spectrophotometry, turbidimetry or nephelometry

**III Separation Methods**

1. Separation of $Fe^{3+}$ and $Ni^{2+}$ using tri-n-butyl phophite (TBP) from HCl medium (Solvent extraction)
2. Determination of cations by paper chromatography; Co(II), Ni(II) and Cu(II)
3. Separation of Fe(III) and Al(III) by column chromatography
4. Separation of $Fe^{3+}$ and $Ni^{2+}$ using strongly basic anion resin.

**SUGGESTED BOOKS**


1.Chemistry Experiments for Instrumental Methods, Donald T Sawyer WilliamR.Hememan et.al John Wiley & Sons 1984.
2.Analytical Chemistry by Gary D.Christian 6th EditionJohn Wiley&Sons Inc New York 1994.
3.A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rdEditionElbs Publication 1969.
4.Vogel's Text Book of Quantitative Inorganic Analysis Jeffery etal 4th edition ElbsPublications 1988.
5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd 2002.
6.Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn.CBS Publishers &Distrbutors1994.
7.Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al New Age Publications 1997.
8. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2ndedn. 1996.


# LABORATORY COURSES (IV Semester)

## Paper CH (IC) 452: Spectroscopic techniques

## Course Objectives

1. Estimate manganese and chromium concentrations using spectrophotometric methods. Simultaneously determine manganese and chromium in mixtures. Determine pKa values of indicators (methyl orange or methyl red). Estimate nickel concentrations using spectrophotometry. Apply Job's Method and Mole ratio Method to determine complex composition in Cu (II)-EDTA and Fe (II)-o-Phen complexes.

2. Determine blood sugar levels using colorimetric methods. Measure blood cholesterol concentration using colorimetry. Estimate creatinine levels using colorimetric techniques. Quantify Paracetamol concentration using colorimetry.
3. Determine Riboflavin concentration using fluorimetry. Quantify Quinine Sulphate concentration using fluorimetric methods.
4. Determine concentrations of Na, K, Ca, and Li using flame photometric techniques.
5. Quantify concentrations of Fe, Mg, Cu, and Pb using atomic absorption spectroscopy.

## Learning Outcomes

1. Students will be able to master quantitative estimation of manganese and chromium. Learn simultaneous determination techniques for mixed samples. Understand pH indicator behavior through pKa determination. Develop proficiency in nickel estimation. Apply Job's Method and Mole ratio Method to analyze complex compositions.
2. Acquire skills to determine blood sugar and cholesterol levels. Learn techniques for measuring creatinine and Paracetamol concentrations.
3. Master the determination of Riboflavin and Quinine Sulphate concentrations using fluorimetry.
4. Develop proficiency in quantifying Na, K, Ca, and Li concentrations using flame photometry.
5. Acquire skills to determine Fe, Mg, Cu, and Pb concentrations using atomic absorption spectroscopy.

**I Spectrophotometry**

1. Estimation of manganese.
2. Estimation of chromium.
3. Simultaneous determination of Manganese and Chromium in a mixture.
4. Determination of pKa of indicator (methyl orange/ methyl red)
5. Estimation of Nickel.
6. Determination of composition of Complex by Job's Method and Mole ratio Method in the following:

(i) Cu(II)-EDTA (ii)Fe(II) - o-Phen

**II Colorimetry**

1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of creatinine
4. Determination of Paracetamol

**III Fluorimetry**

1. Determination of Riboflavin
2. Determination of Quinine Sulphate.

**IV Flame photometry**

1. Determination of Na
2. Determination of K
3. Determination of Ca

4. Determination of Li

**V Atomic Absorption Spectroscopy**

1. Determination of i) Fe, ii) Mg, iii) Cu, iv) Pb.

**SUGGESTED BOOKS**


Text Book of Quantitative Inorganic Analysis Jafferyetal 4th edn. EdnElbs Publication

1. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd EdnElbs Publication 1969.
2. Quantitative Analysis by Day and Underwood Prentice Hall (India) VI Edn.
3. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
4. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers, 2001
5. Medical Laboratory Technology – Mukherjee,McGraw Hills,1988

## SEMESTER-III

**PAPER-I : Synthetic reagents, Advanced NMR, Conformational analysis and ORD**

**UNIT -I : (Synthetic reagents-I)**

**Syllabus:**

**i). Protecting groups:**

a) Protection of alcoholsby ether, silyl ether and ester formation.

b) Protection of 1,2-diols by acetal, ketal and carbonate formation.

c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl,fmoc and triphenyl methyl groups.

d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung)groups.

e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

**ii). Organometallic Reagents:** Preparation and application of the following in organic synthesis: 1) Organolithium 2) Organo copper reagents3) Organoboranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.

**iii). Carbonyl methylenation:**a) Phosphorousylide mediated olefination 1) Witting reaction, 2) Horner-Wordsworth-Emmons reaction.b) Titanium-Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.

**iv). Carbene insertions:** Rh based carbene complexes, cyclopropanations.

**v). C-H Activation:** Introduction, Rh catalysed C-H activation.

**COURSE OUTCOME:**

- In the total synthesis or in any process development, protections and deprotections play an important role.
- *With the reactivity umpolung concept, organometallic reagents are useful in C-C bond formations.
- *In contrast to the conventional methods of generating C=C which involve hard bases, carbonyl methylenation allows an easy C=C formation.
- *Reactions at unexpected positions could be planned with C-H activation.

**LEARNING OUTCOME**

- Importance of protections and deprotections while doing the total and semi synthesis.
- C-C bond formations using organometallic reagents involving reactivity umpolung concept
- Comparison of methods involving C=C formation with hard bases against carbonyl methylenation for an easy C=C formation.
- Reactions at unexpected positions could be planned with C-H activation.

**UNIT -II (Synthetic reagents-II)**

**Syllabus:**

**i).Oxidations:** a) Oxidation of active C-H functions: DDQ and $SeO_2$.b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls:$Cr^{VI}$ oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation

d) Oxidative cleavage of 1,2- diols: Periodic acid and Lead tetra acetate.
**ii). Reductions:** a) Catalytic hydrogenation: Homogenous (Wilkinsons's catalytic hydrogenation)and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c)Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications.e) Electrophilic metal hydrides: $BH_3$, $AlH_3$ and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

**COURSE OUTCOME:**

- Oxidations with new reagents enable the introduction of -OH or C=O group that help in chain lengthening or further chemical manipulations.
- Importance and application of homogenous and heterogenous catalytic hydrogenation.
- Synthetic utility of reductions with electron or hydride additions.
- Reductions involving free radicals and electrophiles.

**LEARNING OUTCOME**

- Oxidations with new reagents enable the introduction of -OH or C=O group that help in chain lengthening or further chemical manipulations.
- Importance and application of homogenous and heterogenous catalytic hydrogenation.
- Synthetic utility of reductions with electron or hydride additions.
- Reductions involving free radicals and electrophiles.

**UNIT-III: ($^{13}$C NMR spectroscopy and 2D NMR spectroscopy)**

**Syllabus:**

i). Introduction**,** Types of $^{13}$Cnmr spectra: undecoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ($^{13}$C, $^{13}$C J) and heteronuclear ($^{13}$C,$^{1}$H J and $^{13}$C, $^{2}$H J) coupling. Applications of $^{13}$C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. $^{13}$C- NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.
**ii). 2D-NMR spectroscopy:** Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY ($^{1}$H-$^{1}$H COSY) , TOCSY (Total Correlation Spectroscopy), HeteroCOSY ($^{1}$H,$^{13}$C COSY,HMQC), long range $^{1}$H,$^{13}$C COSY (HMBC),Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

**COURSE OUTCOME:**

- Interpret 13C chemical shifts and factors affecting them.
- Apply NMR coupling (homonuclear and heteronuclear) to analyze organic compounds.

- Use 13C-NMR for structure determination, stereochemistry, reaction mechanisms, and dynamic processes.
- Apply spectral editing techniques (APT, INEPT, DEPT) effectively.
- Understand principles and types of 2D NMR experiments (COSY, TOCSY, HMQC, HMBC).
- Apply 2D-NMR for determining connectivity, stereochemistry, and long-range interactions in molecules.
- Use advanced techniques like NOESY and 2D-INADEQUATE for detailed structural analysis.

**LEARNING OUTCOME**

- Understanding the interpretation of carbon-13 NMR in identifying the different types of carbons.
- Helps in deciding the carbon skeleton of organic compounds.
- Advantage of 2D-NMR in deciding the stereochemistry and connectivity issues while elucidating the total molecular structure.
- Improved resolution and sensitivity over 1D-NMR makes the task for assigning structure easy.
- Applications of new techniques such as COSY, NOESY, TOCSY, HMQC and HMBC..etc.

**UNIT-IV: Conformational Analysis of Cyclic Systems and ORD**

**Syllabus:**

i). Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5- trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2- halocyclohexanones, cycloheptane . Stereo chemistry of bicyclo[3,3,0]octanes,hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinolineand quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. ( oxidation, $S_N2$ reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

**ii). Optical Rotatory Dispersion (ORD) and CD Spectroscopy:**Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempiricalrules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

**COURSE OUTCOME:**

- Study cyclohexanes, cyclohexanones, and fused ring systems.
- Analyze reactivity and stereochemistry in various organic reactions.

- Investigate conformational structures of piperidines and related compounds.
- Understand factors influencing reactivity of axial and equatorial substituents in cyclohexanes.
- Examine stereochemistry in cyclohexanone ring additions.
- Interpret ORD and CD spectra for optical rotation, circular birefringence, and dichroism.
- Apply rules (e.g., axial haloketone, octant, helicity, exciton chirality) for determining absolute configurations and conformations.

**LEARNING OUTCOME**

- Understanding of the three-dimensional structure and dynamics of cyclic compounds.
- Importance of ring strain, steric interactions, and electronic effects.
- Fundamentals of ORD and its application in determining the absolute configuration of chiral molecules.
- Application od ORD in solving the research problems

## PAPER-II : MODERN ORGANIC SYNTHESIS

### UNIT-I: ASYMMETRIC SYNTHESIS

**Syllabus:**

**Introduction**: Brief revision of classification of stereo selective reactions
**Prostereoisomerism**: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.
**Prochiral nomenclature**: Pro chiraility and Pro-R, Pro-S, Re and Si. Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.
**Analytical methods:** % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.
**Chiral Substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.
**Chiral auxiliary controlled asymmetric synthesis:** α-Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule.
**Chiral reagent controlled asymmetric synthesis:** Asymmetric reductions using BINAL-H. Asymmetric hydroboration using $IPC_2$ BH and $IPCBH_2$.
**Chiral catalyst controlled asymmetric synthesis:**Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphin catalyst.
**Asymmetric aldol reaction:**Diastereoselective aldol reaction (achiral enolate& achiral aldehydes ) its explanation by Zimmerman-Traxel model.

**COURSE OUTCOME:**

- Understand stereo-selective reactions and pro-stereoisomerism.
- Learn topicity in molecules and symmetry criteria for identifying homotopic, stereoheterotopic groups and faces. Understand prochiral nomenclature (Pro-R, Pro-S, Re, Si).
- Explore conditions for achieving stereoselectivity, including symmetry and transition state criteria. Master % enantiomeric excess and diastereomeric ratio determination using techniques like specific rotation, Chiral NMR, chiral derivatizing agents, solvents, shift reagents, and Chiral HPLC.
- Study substrate-controlled asymmetric synthesis (nucleophilic additions, Cram's rule, Felkin-Anh model).
- Explore chiral auxiliary-controlled methods (α-alkylation, Evan's oxazolidinone, 1,4-asymmetric induction, Prelog's rule).
- Learn about chiral reagent-controlled techniques (asymmetric reductions, hydroboration).
- Understand chiral catalyst-controlled methods (Sharpless epoxidation, asymmetric hydrogenations).
- Analyze diastereoselective aldol reactions with achiral enolates and aldehydes using the Zimmerman-Traxel model.

**LEARNING OUTCOME:**

- Principles and mechanisms of stereoselective reactions.
- Understanding the importance of chiral auxiliaries.
- Application of catalysts and enzyme-mediated processes in stereoselective reactions.
- Assessing stereochemical outcomes with NMR and HPLC..

## UNIT-II: SYNTHETIC STRATEGIES

**Syllabus:**

**Introduction:**Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

**Order of events**: S-Salbutamol, Propoxycaine..

**One group C-C and C-X disconnections**: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

**Two group C-C and C-X disconnections :**Introduction .Two group C-X disconnections in 1,1-di functionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds. Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

**Control in carbonyl condensations**:oxanamide and mevalonic acid.

**Strategic bond**: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection

corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis ofRetronecene, longifoline.

**COURSE OUTCOME:**

- Define target, synthon, synthetic equivalent, FGI, and functional group addition.
- Master principles of retrosynthetic analysis, including chemoselectivity, regioselectivity, polarity reversal, and cyclizations.
- Explore linear and convergent synthesis approaches.
- Apply retrosynthesis to compounds like S-Salbutamol and Propoxycaine.
- Learn one-group C-C and C-X disconnections in alcohols, carbonyl compounds, ethers, and sulfides. Study two-group C-C and C-X disconnections, including Diels-Alder reactions, Michael additions, and Robinson annulations.
- Understand strategic bond disconnections in oxanamide and mevalonic acid.
- Apply symmetry, high-yielding steps, and known reactions in retrosynthetic planning. Apply these principles to complex molecules like Retronecene and Longifoline

**LEARNING OUTCOME:**

- Concepts of synthetic strategies in addressing the synthetic problems.
- Various types of disconnections(C-C & C-X) and bond formations.
- Identifying the cheap and commercially available suitable starting materials.
- Development of new procedures for the medicinally and commercially important molecules using strategies.

## UNIT-III: NEW SYNTHETIC REACTIONS

**Syllabus:**

**1). Metal mediated C-C and C-X coupling reactions:**Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwigand Negishi-Kumada coupling reactions.

2). **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurreyreactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.

3). **Multicomponent Reactions:**Ugi,Passerini, Biginelli, Bergman and Mannich reactions.

4). **Ring Formation Reactions:**Pausan-Khand reaction, Nazerov cyclisation.

**5). Click Chemistry:**Click reaction, 1,3-dipolar cycloadditions.

6). **Metathesis:**Grubb's 1$^{st}$ and 2$^{nd}$ generation catalyst, Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications.

7). **Other important synthetic reactions:**Baylis-Hilman reaction,Eschenmoser-Tanabe fragmentation,Mitsunobu reaction,Stork-enamine reaction and Michael reactions.

**COURSE OUTCOME:**

- Introduction of metal catalyzed new C-C and C-X couplings.
- Discussion on Stereoselective olefination methods.
- One-Pot three component or four component reactions and their developments.
- Concept of 1,3-Dipolar cycloadditions in developing five membered ring systems.

- *Development, application and new methods in synthesizing catalysts for Metathesis.

**LEARNING OUTCOME:**

- Introduction of metal catalyzed new C-C and C-X couplings.
- Discussion on Stereoselective olefination methods.
- One-Pot three component or four component reactions and their developments.
- Concept of 1,3-Dipolar cycloadditions in developing five membered ring systems.
- Development, application and new methods in synthesizing catalysts for Metathesis.

## UNIT-IV: NEW TECHNIQUES and CONCEPTS IN ORGANIC SYNTHESIS

**Syllabus:**

1). Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin,synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.
2). Solid phase oligodeoxynucleotide synthesis:Phosphotriester, phosphitetriester and phosphoramidite pathway.
3). Oligosaccharide synthesis:Glycosidation:cylicoxocarbeniumion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.
4). Phase Transfer catalysis: Onium and crwon ethers as PTC.
5). Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.
6). Baldwin Rules:Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavouredcyclisations.
7). Chiron approach in organic synthesis:Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.
8) Determination of absolute configuration: Mosher's method.

**COURSE OUTCOME:**

- Master solid-phase peptide synthesis (SPPS) using commonly used resins like Rink resin, Wang resin, and Ellman resin. Understand synthesis of cross-linked Merrifield resin and drawbacks of SPPS.
- Study glycosidation mechanisms including cyclic oxocarbenium ion, glycosyl donors, and acceptors. Learn Kahne glycosidation, convergent, and linear oligosaccharide synthesis techniques.
- Understand onium and crown ethers as phase transfer catalysts in organic synthesis.
- Explore tandem reactions such as conjugate addition.
- Explore tandem reactions: conjugate addition-aldol, polymerization-cyclization, electrocyclic-Diels Alder reactions.
- Understand Baldwin's rules in cyclization reactions.Apply Chiron approach using natural chiral sources (carbohydrates, amino acids, terpenes). Learn Mosher's method for determining absolute configuration

**LEARNING OUTCOME:**

- Discover and develop new and improved chemical methods.

- Excision or manipulation of functional groups.
- Utility of environmental friendly and sustainable technologies.

## PAPER-III A : BIOORGANIC CHEMISTRY.

## UNIT-I : CARBOHYDRATES

**Syllabus:**

1). Introduction to the importance of Carbohydrates.
2).Types of naturally occuring sugars. Deoxy sugars, aminosugars, branched chain sugars methyl ethers and acid derivatives of sugars.
3). Determination of configuration and determination of ring size of D-glucose and D-Fructose.
4). Conformational analysis of monosaccharides. $^{4}C_{1}$ and $^{1}C_{4}$ conformations of D-glucose.
5). Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement.
6 ) . Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose.
7). Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose.
8). Structure and biological functions of starch, cellulose, glycogenand chitin.
9). Role of sugars in cell to cell recognition, blood groups.

**COURSE OUTCOME:**

- Understand their biological importance in energy, structure, and cell recognition.
- Identify deoxy, amino, branched-chain, methyl ethers, and acid derivatives of sugars.Learn methods to determine configuration and ring size of D-glucose and D-fructose.
- Study key conformations like 4C1 and 1C4 in D-glucose and other monosaccharides.
- Explore reactions specific to six-carbon sugars, including Ferrier rearrangement and Hanesian reactions.
- Understand synthesis methods for amino, halo, and thio sugars. Analyze structures of sucrose and maltose. Examine conformational structures of common disaccharides.
- Explore the structure and functions of starch, cellulose, glycogen, and chitin.
- Understand sugars' roles in cell recognition, blood groups, and other biological processes.

**LEARNING OUTCOME:**

- Understanding the structural features of monosaccharides, disaccharides and polysaccharides.
- Classification of sugars based on the number of sugar units and the type of functional groups.
- Biological significance of carbohydrates as energy depots and structural components.
- Synthetic modifications towards medicinally important analogues.

## UNIT-II : NUCLEIC ACIDS and LIPIDS

**Syllabus:**

**Nucleic acids:** Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

**Lipids:**Introduction and classification of lipids. Stereochemical notation in lipids.Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

**COURSE OUTCOME:**

- Understand nucleotide, nucleoside, base, and sugar structures.
- Master nucleoside and nucleotide synthesis.
- Explain DNA's primary, secondary, and tertiary structures.
- Differentiate mRNA, tRNA, and rRNA functions.
- Comprehend genetic code and DNA fingerprinting.Classify lipids and note stereochemical notation.
- Explain phospholipid and glycolipid synthesis.
- Understand lipid aggregate properties and biological membranes.

**LEARNING OUTCOME**

- Synthesis and retro synthesis of Nucleotides and Nucleosides.
- Chemical composition and folding patterns of DNA and RNA molecules.
- Chemical and biosynthesis of some Lipid molecules

**UNIT-III : PROTEINS and ENZYMES**

**Syllabus:**

**Proteins:** Introduction. Peptide bond, classification and nomenclatue of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins.

**Enzymes:** Definition. Classification based on mode of action. Mechanism of enzyme catalysis- Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity – chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

**COURSE OUTCOME:**

- Understand peptide bonds and classify peptides.
- Analyze amino acid sequences in polypeptides and proteins.
- Describe primary, secondary, and tertiary protein structures.
- Learn peptide synthesis methods.

- Define enzymes and classify them based on their action modes.
- Explore enzyme catalysis mechanisms: Lock and Key, Induced-Fit, and three-point contact.
- Understand enzyme selectivity: chemo-, regio-, diastereo-, and enantioselectivity.
- Study factors affecting enzyme catalysis and enzyme inhibition (reversible and irreversible).
- Examine enzymes' role in organic synthesis and their application when immobilized.

**LEARNING OUTCOME**

- Importance of Biomolecules .
- Various aspects of amino acids and advantage of trans-peptide linkage.
- Primary, secondary, tertiary structures of Proteins.
- Importance of quaternary structure.of proteins to generate enzymes.

## UNIT-IV : COENZYME and VITAMINS

**Syllabus:**

**Coenzymes:** Introduction. Co-factors -co substrates -prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of i). Nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, $NADP^+$ NADPH) ii). Flavin adenine nucleotide FAD, $FADH_2$ and iii) Flavin mononucleotide (FMN, $FMNH_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP)and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

**Vitamins:** Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, $B_1$, and $B_2$. Synthesis of vitamins - $B_6$, C, E and K. Structure of vitamin $B_{12}$.

**COURSE OUTCOME:**

- Understand the role of coenzymes in enzymatic reactions.
- Differentiate between vitamin-derived and metabolite-derived coenzymes.
- Coenzyme A (CoA), TPP, PLP, lipoic acid, biotin, tetrahydrofolate, ubiquinone. NAD+/NADH, NADP+/NADPH, FAD/FADH2, FMN/FMNH2. ATP, ADP, SAM, UDP-sugars.
- Understand their roles in specific biochemical reactions.
- Classify vitamins based on biological importance. Vitamin A, B1, B2, B6, C, E, K, B12.
- Briefly mention structures, functions, and synthesis methods

**LEARNING OUTCOME**

- Coenzymes as group transfer agent and Vitamins as precursors of coenzymes
- Coenzymes and vitamins as cofactors in enzymatic reactions.

- Classification of coenzymes and vitamins based on their chemical structures and biochemical functions.
- Differentiation between water-soluble (C, B) and fat-soluble vitamins (A, D, E, K).
- Coenzymes and vitamins in metabolic pathways and consequences of their deficiencies.

**S**

**PAPER-IIIB : FORENSIC CHEMISTRYand TOXICOLOGY**

**UNIT-I : FORENSIC CHEMISTRY-I**

**Syllabus:**

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methods and instrumental techniques.

Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

**COURSE OUTCOME:**

- Understand the role of forensic chemistry in criminal investigations.
- Identify types of cases and exhibits analyzed.
- Conduct preliminary screening using color and spot tests.
- Use standard methods and instrumental techniques for detailed examinations.
- Qualitatively and quantitatively analyze inorganic and organic materials.

**LEARNING OUTCOME :**

- Understand the role of chemistry in forensic investigations.
- Recognize different types of forensic cases and physical exhibits.

- Perform preliminary screening and presumptive tests using colorimetric and spot tests.
- Apply standard methods and instrumental techniques for forensic analysis.

- Conduct qualitative and quantitative analysis of inorganic and organic materials.
- Analyze specific substances such as fertilizers, insecticides, metals, natural products, and industrial chemicals.

- Identify and interpret chemicals commonly encountered in forensic contexts, including acids, alkalis, explosives, and organic solvents.

## UNIT-II : FORENSIC CHEMISTRY-II

**Syllabus:**

Examination of petroleum products - Distillation and fractionation - various fractions and theircommercial uses - Standard method of analysis of petroleum products – Analysis of petroleumproducts for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires – Causes of fire - Analysis of arsonresidues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments,Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

**COURSE OUTCOME:**

- Understand distillation, fractionation, and commercial uses of various fractions.
- Learn standard methods for analyzing petroleum products, including detection of adulteration.
- Study the chemistry of fire, causes of fires, and techniques for investigating and evaluating fire scenes.
- Analyze arson residues using conventional and instrumental methods.
- Analyze a variety of trace evidence materials (cosmetics, dyes, fibers, paints, oils, chemicals, etc.) using both conventional and instrumental methods.

**LEARNING OUTCOME**:

- Perform distillation and fractionation, identifying fractions and their commercial uses.
- Apply standard methods to analyze for quality, composition, and adulteration.
- Understand the chemistry of fire and conduct fire scene investigations.
- Analyze arson residues using conventional and instrumental methods.
- Identify and analyze trace evidence such as cosmetics, dyes, fibers, paints, and industrial materials.
- Apply techniques to characterize and interpret findings in forensic investigations.
- Gain practical skills in forensic chemistry to contribute effectively to criminal investigations and legal proceedings.
- Apply scientific principles to evaluate evidence and support forensic conclusions.

## UNIT-III : FORENSIC TOXICOLOGY-I

**Syllabus:**

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation oftoxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms ofpoisoning- Toxicological investigation/examination of poisoned death- Interpretationoftoxicologicaldata- Courtroom testimony in toxicological cases.Case Histories.

**COURSE OUTCOME:**

- Understand the history, scope, and roles within toxicology, especially forensic toxicology.
- Classify poisons and recognize different types of poisoning incidents.
- Learn effective methods for collecting, preserving, and storing toxicological samples in fatal and non-fatal poisoning cases.
- Identify signs and symptoms of poisoning and conduct thorough toxicological investigations in suspected poisoning deaths.
- Interpret toxicological data accurately and prepare for courtroom testimony in toxicological cases.
- Study case histories to understand practical applications of toxicological principles.

**LEARNING OUTCOME:**

- Understand the history and scope of toxicology in forensic science.
- Explore the various areas of toxicology and the role of forensic toxicologists.
- Classify poisons and identify different types of poisoning incidents.
- Learn methods for sample collection, preservation, and storage of toxicological exhibits in fatal and survival cases.
- Recognize signs and symptoms of poisoning and their implications in forensic investigations.
- Conduct toxicological examinations and interpret data in cases of suspected poisoning deaths.
- Apply toxicological principles to analyze evidence and support forensic conclusions.
- Prepare for courtroom testimony and understand the role of toxicologists in legal proceedings.

**UNIT-IV : FORENSIC TOXICOLOGY-II**

**Syllabus:**

Principles of Toxicology- Introduction – Pharmacokinetics - Methods of transportation of toxicant- Absorption- Distribution- Storage of toxicants- Redistribution – Metabolism-Oxidation– Reduction – Hydrolysis – Conjugation - Excretion- Other routes of elimination-Toxicokinetics- one and two compartmental model – Toxicodynamics- Spectrum of undesired(toxic) effects- Interaction of chemicals- Tolerance- Dose response relationship- Developmentaland reproductive toxicity- Mutagenicity- Toxicity testing.

**COURSE OUTCOME:**

- Understand core principles and scope of toxicology in assessing chemical effects.
- Learn processes of absorption, distribution, metabolism, and excretion (ADME) of toxicants.

- Study metabolism pathways (oxidation, reduction, hydrolysis, conjugation) and routes of toxicant elimination.
- Compare one-compartment and two-compartment models in toxicant distribution and accumulation.
- Explore spectrum of toxic effects, interactions of chemicals, development of tolerance, and dose-response relationships.
- Analyze developmental/reproductive toxicity, mutagenicity, and methods for toxicity testing

**LEARNING OUTCOME:**

- Understand the basic principles and scope of toxicology.
- Study the absorption, distribution, metabolism, and excretion (ADME) of toxicants.
- Explore methods of transportation, storage, redistribution, and routes of elimination.
- Examine the one and two compartmental models of toxicokinetics.

- Understand toxicodynamics, which encompasses the spectrum of toxic effects and interactions of chemicals.
- Investigate the dose-response relationship and factors influencing tolerance.
- Study developmental, reproductive, and mutagenic toxicity.
- Gain insights into toxicity testing methods and their applications.

## PAPER-IV A : GREEN CHEMISTRY.

### UNIT-I : PRINCIPLES OF GREEN CHEMISTRY

**Syllabus:**

**Green chemistry**: Introduction. Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals ; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization – careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

**COURSE OUTCOME:**

- Understand principles for sustainable chemical processes.
- Apply principles like atom economy, waste prevention, and minimizing hazardous products.
- Select green solvents, ionic liquids, or solvent-free methods.
- Evaluate energy use, including microwaves and ultrasonics in organic synthesis.
- Minimize derivatization and use catalytic reagents over stoichiometric ones.
- Design biodegradable products.
- Prevent chemical accidents and enhance analytical techniques to reduce hazardous substance generation.

**LEARNING OUTCOME:**

- Principles of green chemistry.
- Application of of green chemistry principles in organic synthesis.

## UNIT-II : GREEN SYNTHESIS

**Syllabus:**

i). Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations.
a). Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.
b). Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.
ii)Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound-Cannizaro reaction, Reformatsky reaction and Strecker synthesis.
iii). Organic Synthesis in Green Solvents: introduction.
a). Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and diydroxylationreactions.
b). Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.
iv). Green Catalysts in organic synthesis: introduction
a). Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction
b). Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

**COURSE OUTCOME:**

- Understand principles and benefits of microwave-assisted organic reactions.
- Apply techniques in esterification, rearrangements, Diels-Alder reactions, and solvent-free processes.
- Explore applications in Cannizaro, Reformatsky, and Strecker reactions.
- Learn to perform reactions like Diels-Alder, Heck, and condensations in aqueous phases.
- Apply in Beckmann rearrangement, Suzuki Cross-Coupling, and other reactions.
- Utilize in Williamson ether synthesis and Wittig reactions.
- Apply for microbial oxidations and reductions

**LEARNING OUTCOME:**

- Utility of heat generating process.
- Advantages of Green catalysts.
- Importance of Green solvents

## UNIT-III: ORGANIC NANOMATERIALS

**Syllabus:**

**Introduction**: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation. **Molecular Devices**: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.

**New Carbon family**: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic roperties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes. Structures of aromatics belts, nano car and molecular machines.

**Optoelectronic molecules**: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures) Natural Benzheterazoles and their synthetic modifications as optoelectronic molecules.

**COURSE OUTCOME:**

- Understand 'top-down' and 'bottom-up' nanotechnology approaches. Learn nanomanipulation techniques for precise molecular control.
- Study photochemical devices, liquid crystals, molecular wires, rectifiers, switches, and molecular muscles.Explore their applications in nanotechnology and electronics.
- Classify fullerenes and types of carbon nanotubes (zig-zag, armchair, chiral). Examine growth methods, chemical synthesis, and optoelectronic properties of fullerenes, single-walled CNTs (SWCNTs), multi-walled CNTs (MWCNTs), and graphenes.
- Study aromatic belts, nano cars, and molecular machines. Understand OLED mechanisms and structures. Explore natural benzheterazoles and synthetic modifications for optoelectronic applications.
- Possess a comprehensive understanding of nanotechnology principles and applications, including nanomanipulation and molecular devices.  Be familiar with the growth, synthesis methods, and optoelectronic properties of fullerenes, carbon nanotubes, and graphenes.
- Gain knowledge of optoelectronic molecules like OLEDs and organic solar cells, and their potential applications in electronics and photonics.

**LEARNING OUTCOME:**

- Different types of Nanomaterials such as nanoparticles, nanotubes, nanowires, and nanosheets.
- Methods of their synthesis such as self-assembly, bottom-up synthesis, and functionalization.
- Characterization techniques such as TEM, SEM, AFM, XRD and spectral methods
- Applications in various fields, including electronics, sensors, catalysis, drug delivery, biomedical imaging, and environmental remediation.

## UNIT-IV : SUPRAMOLECULAR CHEMISTRY

**Syllabus:**

I**ntroduction**: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion- π, π-π and Van der Walls interactions),Ionophore and molecular receptors.
**Host-Guest Chemistry**: Lock and key anology, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.
**Self-assembly**: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.
**Enantioselective molecular recognition**: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

**COURSE OUTCOME:**

- Understand essential interactions like ion-ion, ion-dipole, hydrogen bonding, π-π stacking, and van der Waals forces.
- Explore their significance in molecular recognition and assembly.
- Apply the lock and key analogy to molecular recognition.
- Study Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands, and hemicarcerands for their structures, properties, and applications.
- Investigate structures like ladder, polygons, helices, rotaxanes, catenanes, molecular necklaces, dendrimers, and capsules.
- Explore their synthesis, properties, and roles in nanotechnology and drug delivery.
- Study Cyclodextrins, Crown ethers with chiral frameworks, and chiral receptors.
- Examine their applications in selective recognition of chiral molecules

**LEARNING OUTCOME:**

- Principles of Supra Molecular Chemistry.
- Applications of Supra Molecular Chemistry.

## PAPER- IV B : PESTICIDES

### UNIT-I : INTRODUCTION TO PESTICIDES

**Syllabus:**

**Definition** ,Classification and importance of pesticides. **Pest control**: Different methods – chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents. **Biological**–pheremones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants. Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.Moultingharmones-structural formulae and mode of action of ecdysones. Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and

phytoalexins. **Environmental pollution from pesticides**.iv) Integrated pest management. Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

**COURSE OUTCOME:**

- Understand types and importance in agriculture and health.
- Explore insecticides, fungicides, herbicides, rodenticides, fumigants, and insect repellents.
- Study pheromones, juvenile hormones, and microbial-origin compounds as alternatives.
- Discuss sustainable pest control strategies integrating biological, cultural, and chemical methods.
- Analyze pesticide effects and environmental considerations.
- Study pesticide formulations like dusts, granules, powders, emulsions, and aerosols.

**LEARNING OUTCOME:**

- Classification of Insecticides, fungicides, herbicides, rodenticides, fumigants, growth regulators, repellents.
- Essential for crop protection, food security, and economic stability.
- Chemical: Insecticides, fungicides, herbicides, rodenticides, fumigants, growth regulators.
- Biological: Pheromones (sex attractants), insect juvenile hormones (growth regulators), moulting hormones (ecdysteroids), microbial-derived compounds (antibiotics, fungicides).
- Pesticide pollution through soil, water, air contamination from runoff, drift, and improper disposal.
- Sustainable approach combining biological, cultural, and chemical methods to minimize pesticide use.
- Dusts, granules, wettable powders, emulsions, aerosols for effective application.

**UNIT-II : SYNTHETIC INSECTICIDES**

**Syllabus:**

**Organochlorine insecticides**- synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan. **Organophosphorous insecticides** – synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan. **Carbamate insecticides**- synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron. Formulation and residue analysis of organochlorine, organophophorous and carbamate insecticides.

**COURSE OUTCOME:**

- Study methoxychlor, perthane, Dicofol, Heptachlor, Dieldrin, and Endosulfan.
- Understand techniques for formulating and analyzing residues of organochlorine insecticides.

- Explore Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP, and Sachradan.
- Learn methods for formulating and analyzing residues of organophosphorus insecticides.
- Study carbamyl, Furadan, Baygon, Aldicarb, and Zectron.
- Understand formulation techniques and residue analysis methods for carbamate insecticides.

**LEARNING OUTCOME :**

- **Synthesis and Mode of Action:** Includes methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin, and Endosulfan. They act primarily on the nervous system of insects by disrupting neurotransmission.
- **Synthesis and Mode of Action:** Derived from phosphoric acid, examples include phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP, and Sachradan. They inhibit acetylcholinesterase, leading to neurotransmitter accumulation and nerve damage in insects.
- **Synthesis and Mode of Action:** Includes carbamyl, Furadan, Baygon, Aldicarb, and Zectron. They also inhibit acetylcholinesterase but have a shorter duration of action compared to organophosphates.
- **Organochlorine, Organophosphorus, and Carbamate Insecticides:** Various formulations like emulsifiable concentrates, wettable powders, and granules are used. Residue analysis involves methods like chromatography (e.g., GC, HPLC) to detect and quantify residues in environmental and biological samples.

**UNIT-III : NATURAL INSECTICIDESAND HERBICIDES.**

**Syllabus:**

**Insecticides of palnt origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol(Antifeedants). Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrithrelone. **Concept of Bioinsecticides** – Bacillus thiuringiensis. **Concept of pro-insecticides**-structure and mode of action of pro-pheremones and pre-pro-insecticides. **Herbicides** – synthesis,applications and mode of action of the following Aryloxyalkyl carboxylic acid derivative:2,4-D, MCPA,2,4,5-T and 2,4,5-TP.b) Carbamates- propham and chloropham, c)Urea derivatives –Monouron and diuron, d) Aliphatic acids- Dalapon,TCA, e)Aromatic acids -2,3,6-TBA,Dicomba and Amiben, f)Nitrogen heterocyclic dericvatives – Simazine,Atrazine,Amitrole,Maleic hydrazide Diquat and paraquat, g) Phenols- PCP and Dinoseb, h) Benzonitrile compounds.

**COURSE OUTCOME:**

- Gain comprehensive knowledge of plant-derived and synthetic insecticides, herbicides, bioinsecticides, and pro-insecticides.
- Understand synthesis, applications, and modes of action for effective pest and weed management.

- Be prepared for careers in agriculture, environmental sciences, and public health, focusing on sustainable pest control practices.

**LEARNING OUTCOME:**

- **Pyrethrins (I and II):** Derived from chrysanthemum flowers, effective insect nerve disruptors. **Rotenone:** Broad-spectrum insecticide from plants like derris.
- **Nicotine:** Natural insecticide affecting nervous systems.
- **Neem (Azadirachtin):** Effective against insects; structural formula provided.
- **Polygodial and Warbunganol:** Natural antifeedants synthesized to deter insect feeding.
- **Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decamethrin, Pyrethrolone:** Synthetic insecticides based on pyrethrins, enhanced stability.
- **Bacillus thuringiensis (Bt):** Microbial insecticide targeting pests in agriculture.
- **Pro-pheromones and Pre-pro-insecticides:** Convert to active forms within insects, disrupting reproduction or physiology.
- **Synthesis, Applications, and Mode of Action: Aryloxyalkyl Carboxylic Acid Derivatives:** Selective broadleaf weed killers (e.g., 2,4-D, MCPA).
- **Carbamates:** Growth inhibitors (e.g., Propham, Chlorpropham).
- **Aromatic Acids:** Hormone disruptors for broadleaf weeds (e.g., 2,3,6-TBA, Dicamba).
- **Nitrogen Heterocyclic Derivatives:** Photosynthesis or growth inhibitors (e.g., Simazine, Atrazine).
- **Phenols:** Cell membrane disruptors (e.g., PCP, Dinoseb).

**UNIT IV: FUNGICIDES, AND RODENTICIDES.**

**Syllabus:**

**Fungicides** –classification , synthesis application and mode of action of the following classes: **a**)Carbamates **b)**Quinones-chloranil,Dichlone and Benquinox **c)** perchloromethyl mercaptan derivative –captan,folpet,Difolatan and Mesulfan **d)** Benzimidazoles-carbendazim, Benomyl and Thiabandazole

**Rodenticides**, **a)** Anticoagulents-synthesis and application of warfarin, Coumachlor, Vacor, Coumatetrallyl, Dicoumarol and Bromodiolen.**b)** Acute poisons- application of pindone,Ratindan,SodiumFluoroacetate ,Barium fluoroacetate,Antu,Tetramine,pindone and castrix.

**COURSE OUTCOME:**

- Understand different classes including Carbamates, Quinones (chloranil, Dichlone, Benquinox), perchloromethyl mercaptan derivatives (captan, folpet, Difolatan, Mesulfan), and Benzimidazoles (carbendazim, Benomyl, Thiabendazole).
- Study synthesis methods, applications, and modes of action for each fungicide class.
- **Rodenticides: Anticoagulants:** Explore synthesis and applications of warfarin, Coumachlor, Vacor, Coumatetrallyl, Dicoumarol, Bromodiolen.
- **Acute Poisons:** Understand applications of pindone, Ratindan, Sodium Fluoroacetate, Barium fluoroacetate, Antu, Tetramine, Castrix

**LEARNING OUTCOME:**

- **Carbamates:** Inhibit fungal growth through various biochemical pathways.
- **Quinones:** (Chloranil, Dichlone, Benquinox) Disrupt fungal metabolism and cell function.
- **Perchloromethylmercaptan Derivatives:** (Captan, Folpet, Difolatan, Mesulfan) Prevent fungal growth by inhibiting enzyme activity.
- **Benzimidazoles:** (Carbendazim, Benomyl, Thiabendazole) Interfere with fungal cell division and growth.
- **Synthesis and Application:** (e.g., Warfarin, Coumachlor, Vacor, Coumatetralyl, Dicoumarol, Bromadiolone) Inhibit blood clotting in rodents, leading to fatal hemorrhaging
- **Application:** (e.g., Pindone, Ratindan, Sodium Fluoroacetate, Barium Fluoroacetate, Antu, Tetramine, Castrix) Cause rapid death in rodents through various toxic mechanisms.

## LABORATORY COURSE

## PAPER-V : SYNTHESIS OF ORGANIC MOLECULES, ISOLATION OF NATURAL PRODUCTS AND TLC.

**Syllabus: Synthesis of organic molecules, isolation of natural products & TLC**

**a). Laboratory synthesis of the following compounds:** 2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker- Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4- Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ( $NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

**b). Isolation of the following natural products:** Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation),Lycopene from tomatoes.

**c). Thin layer chromatography :**Thin layer chromatography: Determination of purity ( All the above preparations) , monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the $R_f$ values of known standards.

**COURSE OUTCOME:**

- Organic Synthesis: Learn various synthesis methods including Fischer indole, Baker-Venkatraman, Fries reaction, Sandmeyer reaction, Benzillic acid rearrangement, photochemical reactions, Pechman synthesis, Friedel-Crafts, Beckmann rearrangement, reduction, nitration, and others.
- Natural Product Isolation: Master extraction techniques such as solvent extraction, Soxhlet extraction, and steam distillation for isolating Caffeine, Piperine, Eucalyptus oil, and Lycopene from respective natural sources.

- Thin Layer Chromatography (TLC): Utilize TLC for purity assessment of synthesized compounds, monitoring reaction progress, and identifying unknown organic compounds by comparing Rf values with known standards.

**LEARNING OUTCOME:**

- Development of protocols in the laboratory synthesis of synthetically or medicinally important molecules.
- Comprehension over isolation procedures and their application in extracting the active principles from the medicinally important plants.
- Different methods in TLC and its application in checking the progress of a reaction, Purity of the product and isolation of products using Prep TLC.

## PAPER-VI : SEPARATION and IDENTIFICATION OF ORGANIC COMPOUNDS & COLUMN CHROMATOGRAPHY

**Syllabus:**

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of **09** mixtures should be separated and analyzed by these procedures. **Cannizzaro reaction:** 4-Chloro benzaldehyde as substrate and separation of the resulting two component mixture Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed. **Column chromatography**: Separation of a mixture of *ortho* and *para*-nitroanilinesand any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

**COURSE OUTCOME:**

- Separation of Mixtures by Chemical Methods: Utilize solvent ether, 5% aqueous sodium bicarbonate, 5% sodium hydroxide, and dilute hydrochloric acid for separating two-component mixtures.
- Employ chemical methods to separate three-component mixtures.
- Analysis and Identification: Assess purity of components using Thin Layer Chromatography (TLC).
- Identify compounds through systematic study of physical characteristics (melting point/boiling point), elemental analysis (nitrogen, halogens, sulfur), solubility, functional groups, and preparation of crystalline derivatives. Verify identification by referring to literature and known standards.

- Column Chromatography: Separate mixtures like ortho- and para-nitroanilines using silica gel and chloroform as the eluent. Monitor column chromatography using TLC for effective separation and analysis

**LEARNING OUTCOME:**

- Separation of two component mixtures using acid-base properties and solubility in different polar solvents.
- Separation of three component mixtures using acid-base properties and solubility in different polar solvents.
- Checking the purity with TLC
- Derivatization followed by comparison with available literature.
- Demonstration Column chromatography for thebulk separation.

## SEMESTER-IV

## PAPER-I : DRUG DESIGN and DRUG DISCOVERY

### UNIT-I : PRINCIPLES OF DRUG DESIGN and DRUG DISCOVERY.

**Syllabus :**

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

**COURSE OUTCOME:**

- Drug Discovery Process: Understand disease identification, target selection, and bioassay development. Lead Discovery: Learn screening methods for natural products, synthetic libraries, and existing drugs.
- Pharmacokinetics and Pharmacodynamics:Grasp ADME principles and drug-receptor interactions. Drug-Receptor Interaction Theories: Explore theories like Occupancy Theory and Induced-Fit Theory.
- Natural Products: Study their role, pharmacophore concepts, and pruning techniques.
- Drug Design Principles: Understand principles for agonists, antagonists, and enzyme inhibitors. Serendipitous Discoveries: Explore examples like Penicillin and Librium.
- Prodrug Design: Principles behind prodrug development.
- Patents and Clinical Trials: Introduction to drug patents and clinical trial phases.

- Application: Apply knowledge to understand trends and prepare for careers in pharmaceutical research.

**LEARNING OUTCOME:**

- Principles of drug design and drug discovery.
- Concepts of lead optimisation and modification.
- Clinical trials and patent filing.

**UNIT-II : LEAD MODIFICATION and SAR STUDIES.**

**Syllabus :**

Lead modification strategies, Bioisosterism, variation of alkyl substituents,chain homologation and branching, variation of aromatic substituents,extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead.Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs,benzodiazepines, and taxol analogs.

**COURSE OUTCOME:**

- Lead Modification Strategies: Learn diverse strategies like bioisosterism, alkyl and aromatic substituent variations, ring modifications, and simplification.
- Application in Drug Discovery: Apply SAR principles to discover and optimize drugs such as Oxaminquine, Salbutamol, Cimitidine, and Captopril.
- Analysis of Drug Classes: Analyze SAR in sulfa drugs, benzodiazepines, and Taxol analogs for understanding structure-activity relationships.
- Interpretation and Application: Interpret SAR data to predict drug efficacy, potency, and safety, fostering critical thinking in drug design.
- Integration and Preparation: Integrate SAR principles into drug discovery contexts, preparing for careers in pharmaceutical research and development.

**LEARNING OUTCOME:**

- Strategies in Lead modifications to develop potentially putative molecules.
- Case studies on discoveries of medicinally important molecules.
- Application of SAR in development of commercially important molecules.

**UNIT-III: QSAR & COMPUTER-AIDED DRUG DESIGN (CADD).**

**Syllabus :**

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants($\sigma$), lipophilicity constant($\pi$), steric effects and Taft's constant, linear and nonlinear relationship between biological activityLipophilicity Substituent constants. Lipinski rule

of five. Hansch analysis, Craig's plot,Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

**Computer aided drug design:** Introduction, active site, allosteric binding site,use of grids in docking , rigid docking , flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

**COURSE OUTCOME:**

- QSAR: Understand physicochemical properties like pKa, electronic effects (σ), lipophilicity (π), and steric effects.. Analyze relationships between these properties and biological activity.
- Apply Lipinski's Rule of Five, Hansch analysis, and case studies like pyranenamine and Crizotinib design.
- Learn principles of active site identification and allosteric binding sites. Utilize docking techniques such as rigid, flexible, and induced fit docking with computational grids.
- Differentiate between structure-based and ligand-based drug design, including de novo design principles.
- Application and Integration: Apply QSAR and CADD tools to predict and optimize drug candidates. Develop problem-solving skills for drug design challenges using computational approaches.

**LEARNING OUTCOME:**

- Use of computational tools in drug discovery.
- Validate of QSAR models such as molecular docking and virtual screening techniques.
- Optimizing the lead compounds with the integration of theoretical and practical skills to predict biological activity,

**UNIT-IV : <u>COMBINATORIAL SYNTHESIS.</u>**

**Syllabus :**

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

**COURSE OUTCOME:**

- Understand combinatorial chemistry principles and their applications.

- Evaluate combinatorial libraries and synthesis technologies.
- Master solid phase synthesis techniques and resin types.
- Apply parallel synthesis methods like Haughton's tea bag and automated synthesis.
- Implement mixed combinatorial synthesis principles such as Furka's mix and split.
- Use deconvolution methods for structure determination.
- Analyze examples of successful combinatorial chemistry applications.
- Design strategies for planning combinatorial synthesis, including automation.
- Integrate high throughput screening with combinatorial approaches for drug discovery.

**LEARNING OUTCOME:**

- Principles of combinatorial chemistry, including the design, synthesis.
- Analysis of large chemical libraries.
- High-throughput techniques, automation, and the application of combinatorial methods in drug discovery and material science.

**PAPER-II: DRUG SYNTHESIS and MECHANISM OF ACTION**

**UNIT-I : DRUGS ACTING ON METABOLIC PROCESS, CELL WALL and SPECIFIC ENZYMES.**

**Syllabus :**

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a). Drugs acting on metabolic process: Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone. Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism
b). Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors- Structural formulae and mode of action of clavulanic acid and sulbactum
c). Drugs acting on specific enzymes: $H^+/K^+$ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

**COURSE OUTCOME:**

- Understand mechanisms of drug action on macromolecular targets (carbohydrates, proteins, lipids, nucleic acids) and classify drugs based on enzyme inhibition types.
- Explain antifolates' discovery and mechanisms of action, including sulphonamides and diaminopyrimidines like trimethoprim.
- Describe the structure of bacterial cell walls and mechanisms of action for β-lactam antibiotics (penicillins, cephalosporins), with a focus on synthesis methods.
- Analyze resistance mechanisms to penicillins and discuss broad-spectrum penicillins and β-lactamase inhibitors like clavulanic acid and sulbactam.

- Explore specific enzyme inhibitors such as H+/K+-ATPase inhibitors (e.g., Omeprazole) and Carbonic Anhydrase inhibitors (e.g., Acetazolamide), including their synthesis and mechanisms of action.
- Evaluate the clinical relevance and therapeutic applications of drugs targeting these pathways in treating various diseases.

**LEARNING OUTCOME:**

- Basic concepts on drug interaction with macromolecular targets.
- Introduction of agonist and antagonist concept.
- Discoveries on sulfonamides, penicillins and the development of their synthetic analogues.
- Synergistic aspects in developing broad spectrum antibacterials.

**UNIT-II : DRUGS ACTING ON GENETIC MATERIAL and IMMUNE SYSTEMS**

**Syllabus :**

Drugs acting on genetic material:Introduction, classification and mechanism of action.

a). DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.
b). DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.
c). DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.
d). DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.
e). DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.
f). Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.
g). Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin
h).Drugs acting on immune system: Introduction to immune system. (i). Immunosupressing agent- structural formula of Cyclosporin. ( i i ) Immunoenhancers-use of vaccines and strucrural formula of levamisol.

**COURSE OUTCOME:**

- Understand drugs targeting genetic material, including DNA-intercalating agents, DNA-binding agents, DNA-alkylators, DNA-polymerase inhibitors, DNA-topoisomerase inhibitors, inhibitors of transcribing enzymes, and translation process inhibitors.
- Analyze the synthesis methods, mechanisms of action, and clinical applications of key drugs such as Daunomycin, Adriamycin, Chloroquine, Metronidazole, Cyclophosphamide, Acyclovir, Ciprofloxacin, Rifampicin, Erythromycin, Streptomycin, and Chloromycetin.

- Discuss the immune system's components and their interactions with drugs, covering immunosuppressing agents like Cyclosporin and immunoenhancers such as vaccines and Levamisole.
- Evaluate the therapeutic significance and clinical implications of these drugs in treating various diseases, including cancer, infections (bacterial, viral, protozoal), tuberculosis, and immune-related disorders.
- Present and discuss findings effectively, demonstrating understanding through oral presentations and written analyses of case studies and research in the field.

**LEARNING OUTCOME:**

- Drugs acting on genetic materials.
- Drugs acting on the immune system.
- Biological activity studies

**UNIT-III : DRUGS ACTING ON RECEPTORS and ION CHANNELS**

**Syllabus :**

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

i). Drugs acting on receptors:

a). Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin. β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.
b). Cholinergic-receptors: Introduction and classification.Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
c). Dopamine receptors: Introduction and classification.Dopamine-receptoragonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e)Histamine receptors:Introduction and classification.Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine and Ranitidine.
f). Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen

g). Drugs acting on ion channels: Introduction to ion channels, drugs acting on $Ca^{2+}$, $Na^{+}$ and $Cl^{-}$ channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

**COURSE OUTCOME:**

- Understand the nervous system, including neuron structure and neurotransmission fundamentals.
- Define and provide examples of agonists, antagonists, neurotransmitters, and receptors.
- Explore various types of receptors and their pharmacological agents.
- Study drugs targeting ion channels (Ca2+, Na+, Cl-) and their mechanisms of action- Discuss drugs like Tetracaine, Nifedipine, Diltiazem, and 4-Aminopyridine.
- Apply knowledge to analyze drug mechanisms, synthesis methods, and clinical applications in treating neurological, cardiovascular, respiratory, and endocrine disorders.
- Communicate effectively through oral presentations and written reports on drugs acting on receptors and ion channels.

**LEARNING OUTCOME:**

- Drugs interact with specific receptors and ion channels.
- Importance of Ion-channels.
- Mechanisms of drug action and how different drugs produce their effects.

**UNIT-IV : CHIRAL DRUGS**

**Syllabus :**

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion. Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetrazine, 2S-Verapamil, S,S-Ethambutol , (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S-Enalaprilate.

**COURSE OUTCOME:**

- Understand the importance of chiral drugs in pharmacology, including concepts like the Three-Point Contact Model, Eutomer, Distomer, Eudesmic ratio, and Pfeiffer's rule.
- Analyze the role of chirality in biological activity, categorizing Distomers based on their effects: no side effects, undesirable side effects, independent therapeutic value of both isomers, therapeutic advantages of combination products, and metabolic chirality inversion.

- Study specific chiral drugs, their synthesis methods, and pharmacological activities, including examples like S-Ibuprofen, S-Metoprolol, Ritonavir (Ininavir sulfate), Levocetirizine, and others.
- Apply knowledge to assess the impact of chirality on drug development, efficacy, safety, and clinical practice.
- Communicate findings effectively through written reports and oral presentations, evaluating current research trends and future prospects in chiral drug development.

**LEARNING OUTCOME:**

- Importance of Chiral drugs and their synthetic methods.
- Details of aspects of chiral drugs configuration and pharmacological activity.

## PAPER-III A : ADVANCED HETEROCYCLIC CHEMISTRY

### UNIT-I : NON-AROMATIC HETEROCYCLICS and AROMATICITY

**Syllabus :**

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanesandthietanes

**Aromaticity**: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

**COURSE OUTCOME:**

- Understand Nonaromatic Heterocyclics: Explore various types of strains, interactions, and conformational aspects in nonaromatic heterocycles.
- Analyze the synthesis, reactivity, and importance of ring systems such as azirines, aziridines, oxiranes, thiiranes, diazirenes, diaziridines, oxaziridines, azetidines, oxetanes, and thietanes.
- Aromaticity Concepts: Introduce aromatic and antiaromatic compounds. Define the criteria for aromaticity, including Huckel's rule (4n+2 electrons) for benzene and related compounds.
- Discuss examples like cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene, and annulenes.
- Apply Knowledge to Analysis and Prediction: Apply aromaticity rules to predict stability and reactivity of aromatic and antiaromatic compounds. Discuss the significance of aromaticity in organic chemistry, particularly in drug design and material science.
- Critically Evaluate and Apply Concepts: Critically evaluate experimental data and literature on nonaromatic heterocyclics and aromatic compounds. Apply theoretical

principles to solve problems related to ring strain, conformational analysis, and aromaticity in complex molecules.

**LEARNING OUTCOME:**

- Differentiate between aromatic and non-aromatic heterocycles.
- Criteria for aromaticity.
- Non-aromatic heterocycles and explain their reactivity patterns.
- Synthetic methods used to prepare non-aromatic heterocyclic compounds.
- Physical and chemical properties of non-aromatic heterocycles, such as solubility, stability, and biological activity.
- Highlight recent advances in the synthesis and application of non-aromatic heterocyclic compounds

## UNIT-II : FIVE and SIX MEMBERED HETEROCYCLICS WITH TWO HETERO ATOMS

**Syllabus :**

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole,benzoxazole and benzthiazole.

**COURSE OUTCOME:**

- Understand Synthesis and Reactivity: Master synthesis methods for heterocycles like pyrazole, imidazole, oxazole, thiazole, isoxazole, isothiazole, pyridazine, pyrimidine, pyrazine, oxazine, thiazine, benzimidazole, benzoxazole, and benzothiazole.
- Analyze reactivity patterns, including nucleophilic/electrophilic substitutions and functional group transformations.
- Evaluate Aromaticity: - Define aromaticity and apply Huckel's rule to assess aromatic stability in heterocyclic systems. Compare aromatic and non-aromatic properties within these compounds.
- Assess Applications: Discuss pharmaceutical, medicinal, and industrial uses of heterocyclic compounds. Evaluate the impact of structure on biological activity and material properties.

**LEARNING OUTCOME:**

- Synthesis and reactivity of Five membered heterocyclic with two hetero atoms.
- Synthesis and reactivity of Six membered heterocyclic with two hetero atoms.
- Synthesis and reactivity of Benzofused five membered heterocyclic with two hetero atoms.

## UNIT-III : HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS

**Syllabus :**

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.

**COURSE OUTCOME:**

- Acquire proficiency in synthesizing diverse heterocycles like 1,2,3-triazoles, 1,2,4-triazoles, tetrazoles, oxadiazoles, thiadiazoles, triazines, and tetrazines. Analyze reactivity patterns and functional group transformations in these heterocycles.
- Understand Aromaticity: Define and apply aromaticity principles to assess stability in complex heterocyclic systems. Differentiate between aromatic and non-aromatic properties within these compounds.
- Evaluate Applications: Discuss pharmaceutical, medicinal, and industrial uses of heterocyclic compounds with multiple heteroatoms. Assess their role in drug discovery, materials science, and related fields.
- Apply Knowledge in Problem-Solving: Solve theoretical and practical problems related to synthesis, reactivity, and aromaticity of complex heterocyclics.

**LEARNING OUTCOME:**

- Synthesis and reactivity of Five membered heterocyclic with more than two hetero atoms.
- Synthesis and reactivity of Six membered heterocyclic with more than two hetero atoms.
- Synthesis and important of Purines, pteridines and caffeines.

## UNIT-IV : LARGER RING and OTHER HETEROCYCLICS

**Syllabus :**

Synthesis, structure, stability and reactivity ofAzepines, Oxepines and Thiepines. Synthesis of Diazepines rearrangements of 1,2 - diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes,Phospholesand Boroles.

**COURSE OUTCOME:**

- Acquire proficiency in synthesizing larger ring heterocycles such as azepines, oxepines, thiepines, diazepines, benzoazepines, benzodiazepines, benzooxepines, benzothiepines, azocines, and azonines. Analyze reactivity patterns and key reactions, including rearrangements and functional group transformations.

- Evaluate the structural characteristics and stability factors of each heterocyclic compound. - Discuss the impact of ring size, substitution patterns, and heteroatoms on stability and reactivity.
- Study synthesis routes and applications of selenophenes, tellurophenes, phospholes, and boroles in organic electronics, materials science, and catalysis.

**LEARNING OUTCOME:**

- Concept of ring strain in larger ring heterocycles and influence on their stability.
- Structural diversity and geometric variations.
- Conformational preferences and reactivity with angle strain, torsional strain, and steric hindrance.
- Synthetic methods for ring contractions and expansions

## PAPER-IIIB : ORGANIC POLYMERS, DYES AND PIGMENTS.

### UNIT-I : ORGANIC POLYMERS-I

**Syllabus:**

Introduction, Classification of Polymers – according to origin, structure, intermolecular interactions. Types of polymerization – addition, condensation, radical, ionic and coplymerization with mechanism, Ziegler-Natta polymerization with mechanism. Stereochemistry of polymers, Plasticity – types of plastics. Molecular mass of polymers. Resins and plastics – Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate)and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers, polyurethanes and epoxide polymers with examples. Natural and synthetic rubbers.

**COURSE OUTCOME:**

- Classify polymers based on origin, structure, and intermolecular interactions. Explain polymerization types including addition, condensation, radical, ionic, and copolymerization, with focus on mechanisms and industrial applications.
- Describe Ziegler-Natta polymerization and its role in synthesizing stereospecific polymers. Discuss polymer stereochemistry, including tacticity variations. Analyze molecular mass distribution and its impact on polymer properties.
- Identify plastics such as polystyrene, styrene copolymers, poly(vinyl chloride/vinyl acetate), acrylics, polyesters, phenol-formaldehyde, polyurethanes, and epoxides. Investigate natural rubber and synthetic rubbers, including vulcanization processes.

**LEARNING OUTCOME:**

- Analyze polymer properties by structure and origin.
- Understand polymerization mechanisms.
- Identify types of plastics and their uses.
- Recognize rubber roles in industries.

## UNIT-II : ORGANIC POLYMERS – II

**Syllabus:**

a). Functional polymers : Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.

i) Photoconductive polymers: Liquid crystal polymers, smectoc, nematicamd cholesteric structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.
ii) Smart materials: Uses in sensing device and communication networks.
iii)Biodegradable polymers: Definition, classification. Brief description polyhydroxyalkanoates, polycaprolactones, polyactic, polyvinyl alcohol and their applications.
b) Membranes: Filtration, micro, ultra, nano filtration. Separation of gases-Permeselectivity and gas permeability representative polymers. Liquid separation-dialysis, electroosmosis and reverse osmosis.
c) Fire retarding polymers and photonic polymers.
Polymers in biomedical application, artificial organs and controlled drug delivery.

**COURSE OUTCOME:**

- Explain electrically conducting polymers (polyanilines, polypyrroles, polyacetylenes, polythiophenes) and their applications. Discuss photoconductive polymers, including liquid crystal polymers and ion-exchange polymers (cationic and anionic).
- Explore smart materials used in sensing devices and communication networks. Define and classify biodegradable polymers and their applications.
- Analyze membrane processes like filtration (micro, ultra, nano), and separation of gases and liquids (permselectivity, gas permeability, dialysis, electroosmosis, reverse osmosis). Explore fire-retardant polymers, photonic polymers, and their applications.

**LEARNING OUTCOME:**

- This topic provides a comprehensive understanding of advanced polymer applications, from functional and smart materials.
- Specialized uses in membranes, fire retardancy, photonics, and biomedical fields.
- Gain insights into cutting-edge technologies and sustainable practices in polymer science and engineering.
- Preparing them for roles in research, development, and innovation in various industries.

## UNIT-III : DYES – I

**Syllabus:**

Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes[malachite green, rosaniline, para aniline

blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

**COURSE OUTCOME**

- Define synthetic dyes and classify them based on their chemical structure and properties. - Explain the nomenclature system used for synthetic dyes.
- Discuss the relationship between color and molecular structure, including chromophores and auxochromes. Explain historical theories such as Witt's, Armstrong's, Baeyer's, Nietzki's, Watson's, and modern theories including Valence Bond Theory and Molecular Orbital Theory.
- Analyze the chemistry and synthesis methods of triphenyl methane dyes (e.g., malachite green, rosaniline, crystal violet), hydroxytriphenyl methane dyes, Aurin, and chrome violet. Explore the types and synthesis of azo dyes, including acidic and basic azo dyes, mono, di, tri, and poly azo dyes.
- Study natural dyes such as alizarin, quinazarin, and indigo, including their structure determination and synthesis methods.
- Apply theoretical understanding to practical scenarios involving dye synthesis, characterization, and application. Evaluate the suitability of different dye types for specific industrial and artistic applications.

**LEARNING OUTCOME:**

- Equips learners with a deep understanding of synthetic dyes with their theories.
- Understands chemical structure, synthesis methods, and applications in diverse industries.
- Prepares them for roles in research, development, and application of dyes in fields such as textiles, materials science, and biotechnology.

**UNIT-IV : DYES–II AND PIGMENTS**

**Syllabus:**

Interaction of organic molecules with electromagnetic radiation. Energy diagram. Activation and deactivation of organic molecules by light. Fluorescence and delayed fluorescence. Effect of molecular structure on fluorescence. General properties of fluorescent dyes and their requirements. Triplet-triplet absorption of organic molecules. Fluorescent quantum yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons. and Fluorescent heteroaromatic compounds.

a) **Introduction to laser dyes**. Synthesis of Oligophenylenes. Oxazoles and benzoxzoles. Stilbenoid compoundsCoumarin laser dyes, Rhodamine laser dyes.

b) **Pigments:** Introduction, Structures of Porphyrins , Bile pigments. Synthesis of

Haemin and Chlorophyll. Synthetic pigments – preparation of phthalocyanines.

**COURSE OUTCOME:**

c) Explain the interaction of organic molecules with light, including fluorescence and delayed fluorescence. - Analyze how molecular structure affects fluorescence properties and quantum yields.
d) Study the synthesis of fluorescent aromatic hydrocarbons and heteroaromatic compounds. Introduce laser dyes and their synthesis, including oligophenylenes, oxazoles, benzoxazoles, stilbenoids, coumarins, and rhodamines.
e) Discuss the structures and synthesis of natural pigments like porphyrins, bile pigments, haemin, and chlorophyll. Explore synthetic pigments, focusing on the preparation of phthalocyanines.
f) Apply theoretical understanding to practical scenarios involving the application and development of fluorescence dyes, laser dyes, and pigments.

**LEARNING OUTCOME:**

- Understanding of the interaction of organic molecules with light, fluorescence, triplet-triplet absorption, fluorescent dyes, laser dyes, and pigments.
- Advanced studies and applications in fields such as photonics, materials science, biomedical imaging, and optical technologies.

## PAPER-IV A: ADVANCED NATURAL PRODUCTS

### UNIT-I : BIOSYNTHESIS OF NATURAL PRODUCTS

**Syllabus :**

Biosynthesis of secondary metabolites: Introduction,Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism.

Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods.Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono,sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

**COURSE OUTCOME:**

- Differentiate laboratory synthesis from biosynthesis of natural products. Methods to determine biosynthetic mechanisms, including isotopic labeling and precursor identification.
- Measure isotopic incorporation using absolute and specific methods- Use chemical degradation and spectral methods to identify label positions in natural products.

- Acetate-Malonate Pathway: Learn aromatic compound biosynthesis. Shikimic Acid Pathway: Study amino acids (phenylalanine, tyrosine, tryptophan), flavonoids, and morphine alkaloid biosynthesis.
- Mevalonic Acid Pathway: Examine terpene (mono-, sesqui-, di-, tri-), carotenoid, and steroid (e.g., cholesterol) biosynthesis.
- Relate biosynthetic pathways to biological functions and ecological roles.
- .Discuss regulatory mechanisms, enzymatic reactions, and structural diversity in natural product biosynthesis.

**LEARNING OUTCOME:**

- Biosynthesis of natural products.
- Major biosynthetic pathways such as Acetate-Melonate, Shikimic acid and Mevalonic acid pathway.
- Biosynthesis of Aromatic Compounds by Acetate-Melonate pathway and Morphine by Shikimic acid pathway.
- Biosynthesis of terpenoid, cholesterol, carotenoid and flavonoid by Mevalonic acid pathway

**UNIT-II : :- <u>STRUCTURE DETERMINATION OF NATURAL PRODUCTS-I</u>**

**Syllabus :**

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

**COURSE OUTCOME:**

- Proficiently use NMR spectroscopy, mass spectrometry, and infrared spectroscopy for structure determination. Apply chromatographic techniques effectively in analyzing natural products.
- Interpret spectroscopic data to determine structures and stereochemistry of complex natural products like morphine, reserpine, abietic acid, cholesterol, and rotenone.
- Understand the role of X-ray crystallography and computational chemistry in confirming molecular structures. Explore modern methods such as chiroptical spectroscopy for structural elucidation.
- Analyze and interpret experimental data from spectroscopic analyses and chromatographic separations.

**LEARNING OUTCOME:**

- Structure Determination by Chemical Methods of Natural Products.
- Elucidation of molecular structures with degradative methods and derivatization methods.
- Emphasis on retrosynthetic analysis, chiral synthesis, and total synthesis of natural products.

## UNIT-III: STRUCTURE DETERMINATION OF NATURAL PRODUCTS-II

**Syllabus :**

Spectroscopic techniques IR, UV, $^{1}$Hnmr, $^{13}$Cnmr, COSY, HETEROCOSY, NOESY, 2D- INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

**Study of the following solved problems:** Mass, IR, $^{1}$H, $^{13}$C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of **menthol**, APT of **apparicine**,

Heteronuclear 2D-J resolved spectrum of **stricticine**,NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of ***α*-picoline** and ***β*-methyl tetrahydran furan**.

**COURSE OUTCOME:**

- Proficiently utilize IR, UV, 1H-NMR, 13C-NMR, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE, and MS techniques for identifying and elucidating structures of natural products like flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, and isoquinolines.
- Analyze and interpret mass spectrometry, infrared, and NMR (1H, 13C) spectra using advanced methods such as HOMOCOSY, HECTOR, DEPT, NOE, and 2D-INADEQUATE for compounds including geraniol, menthol, apparicine, stricticine, buxaquamarine, strictanol, α-picoline, and β-methyl tetrahydrofuran.
- Understand and apply HETEROCOSY for heteronuclear correlations and NOESY for nuclear Overhauser effects to deduce structural connectivity

**LEARNING OUTCOME:**

- Application of spectroscopic techniques such as NMR, MS, IR, UV-Vis spectroscopy, and HPLC, GC in structure determination.
- Structural elucidation by spectral methods of alkaloids, terpenoids, polyphenols, and other secondary metabolites.
- Verifying the purity of compounds, identifying potential impurities or degradation products,

## UNIT-IV : TOTAL STEREOSELECTIVE SYNTHESIS

**Syllabus :**

Nicalou's synthesis of Dynemicin A , Corey's synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

**COURSE OUTCOME:**

- Total synthesis methods for complex natural products such as Dynemicin A, prostaglandins (E2, F2α), paeoriflorin, L-hexoses, taxol, indolizomycin, menthol, and biotin.
- Examine detailed synthetic routes and key reactions used in each synthesis. Discuss stereochemistry principles and strategic bond formations for achieving stereoselectivity.
- Evaluate challenges in natural product synthesis and innovative strategies to overcome them.
- Use retrosynthetic analysis to plan synthetic routes. Apply protecting group strategies, stereoselective reactions, and functional group manipulations.
- Evaluate efficiency, scalability, and environmental impact of synthetic methodologies. Compare synthetic approaches based on yield, selectivity, and feasibility.

**LEARNING OUTCOME:**

- Advantage of literature survey in trouble shooting difficult synthetic problems.
- Development of new catalysts, reagents or protocols in the customized synthesis of natural products.
- Application of concepts of synthetic organic chemistry in the development of procedures for existing medicinally or commercially important molecules.

## PAPER-IV B : BIOPHARMACEUTICS AND PHARMACODYNAMICS.

## UNIT-I : PHARMACOKINETICS.

**Syllabus:**

Introduction and importance of ADME studies of drugs. Routes of administration i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability. ii)Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding. iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs ( phase I and phase II reactions) iv)Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

**COURSE OUTCOME:**

- Recognize the significance of ADME (Absorption, Distribution, Metabolism, Excretion) studies in drug development and therapeutic effectiveness.
- Routes of Administration:Describe various routes of drug administration and their impact on drug absorption, distribution, metabolism, and elimination.
- Absorption: Explain drug absorption, including physicochemical factors such as pH partition and drug dissolution. Discuss methods used to assess drug absorption and determine bioavailability.
- Distribution: Define apparent volume of drug distribution and factors influencing drug distribution. Explain plasma protein binding and its role in drug distribution dynamics.
- Metabolism: Identify drug metabolism sites and metabolic rate constants. Discuss drug bioactivation and biotransformation via phase I and phase II reactions.
- Elimination:Define drug elimination processes and concepts like elimination rate constant, half-life, and clearance.

**LEARNING OUTCOME:**

- Understand the importance of ADME studies in drug development for optimizing efficacy and safety.
- Routes of Administration, Absorption : Definition, Understand drug absorption and its role in pharmacokinetics.

- Factors Affecting Absorption: Explore pH partition hypothesis, drug dissolution, and methods for determining absorption, Bioavailability, Volume of Distribution, Factors Influencing Distribution, Metabolism-Sites and Reactions: Identify major sites of drug metabolism (e.g., liver) and phases of biotransformation (phase I and II reactions).
- Metabolic Rate: Understand the metabolic rate constant and implications for drug clearance and elimination- Types and Concepts.

**UNIT-II : PHARMACODYNAMICS.**

**Syllabus:**

Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two-statereceptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

**COURSE OUTCOME:**

- Learn the fundamentals of pharmacodynamics, focusing on how drugs interact with targets in the body. Grasp the concept of drug targets, particularly receptors, and the principles of receptor-ligand interactions.
- Signal Transduction Mechanisms:Describe receptor families and their diverse signal transduction mechanisms, including channel-linked proteins, G-protein coupled receptors (GPCRs), and kinase-linked receptors.

- Concentration-Response Relationship: Analyze concentration-response relationships and interpret dose-response curves to understand how drug concentrations influence pharmacological effects.
- Apply pharmacodynamic principles to predict drug effects and assess drug efficacy and potency based on pharmacological profiles

**LEARNING OUTCOME:**

- Understanding Drug Action: Grasp the fundamental principles of how drugs interact with specific targets in the body.

- Receptor Concept: Define receptors as molecular entities that mediate drug effects by binding and initiating biochemical responses.
- Pharmacological Binding Terms-Agonists and Antagonists, Two-State Receptor Model-concept and appliocation.

- Structure and Signal Transduction Mechanisms: Channel-Linked Proteins, G-Protein Coupled Receptors, and Their RoleKinase-Linked Receptors and Receptors Regulating Gene Transcription, Kinase-Linked Receptors
- Theories of Concentration-Response Relationship and Dose-Response Curves

## UNIT-III : PRINCIPLES OF THERAPEUTICS

**Syllabus:**

Plasma Drug concentration vs Time profile,Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plama concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

**COURSE OUTCOME:**

- Interpret plasma drug concentration vs. time profiles and key pharmacokinetic terms like MEC, MSC, MTC, and AUC. Analyze peak plasma concentration, time to peak, and therapeutic range for effective drug therapy.
- Dosage Regimen Design: Design dosage regimens including dose size, frequency, and considerations for drug accumulation during multiple doses.
- Calculate loading and maintenance doses to achieve steady-state concentration and maintain drugs within therapeutic ranges. Modify dosage regimens for obese patients, neonates, children, elderly, and those with hepatic or renal diseases.

Safety and Efficacy: Understand LD50 and ED50 concepts and their implications for drug safety and efficacy

**LEARNING OUTCOME:**

- Plasma Drug Concentration vs Time Profile: Definition and Explanation of Terms: MEC, MSC, MTC. LD50 and ED50, Therapeutic Objective.
- Dosage Regimen Design, Loading Dose and Maintenance Dose, Modification to Dosage Regimen.
- Application of pharmacokinetic principles in clinical practice, ensuring safe and effective drug therapy tailored to individual patient need.

## UNIT-IV : DRUG INTERACTIONS

**Syllabus:**

Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol( Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking( Theophylline, Diazepam, a Tri cyclic antidepressants), food ( Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.

**COURSE OUTCOME:**

- Classify drug interactions into pharmacokinetic (PK) and pharmacodynamic (PD) categories.
- Explain how interactions alter drug absorption, distribution, metabolism, and excretion.
- Analyze how drugs affect each other through changes in absorption, distribution, metabolism, and excretion processes.
- Pharmacodynamic Interactions: Describe antagonistic and synergistic effects of drug combinations. Discuss interactions impacting electrolyte levels, adrenergic system function, and receptor interactions.
- External Factors and Drug Interactions: Evaluate the influence of alcohol, smoking, and food on drug action across various medication classes.

**LEARNING OUTCOME:**

- Introduction to Drug Interactions**,** Classification of Drug Interactions**.**
- Mechanisms of Drug Interactions: Pharmacokinetic Interactions**,** Pharmacodynamic Interactions.
- Influence of Alcohol, Smoking, and Food on Drug Action

## LABORATORY COURSE WORK

## PAPER-V : SPECTRAL INTERPRETATION and CHEMISTRY SOFTWARE PROGRAMS

**Syllabus:**

1. Identification of unknown organic compounds by interpretation of IR, UV, $^{1}H$ -NMR, $^{13}C$ NMR, and mass spectral data( two examples with 2D-NMR). A minimum of 30 representative examples should be studied.

**2. Chemistry software programmes:** Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

**3.**

**COURSE OUTCOME:**

- Spectral Interpretation Mastery: Ability to identify unknown organic compounds using IR, UV, 1H-NMR, 13C NMR, and mass spectral data, including 2D-NMR.
- Software Proficiency: Competence in using ChemDraw for chemical structure and reaction drawing, ACD/Id NMR Processor for spectral analysis, and Excel for graphing and possibly molecular docking.
- Application Skills: Applying knowledge to solve organic compound identification problems and understanding molecular structure-function relationships.

**LEARNING OUTCOME:**

- Application of all spectral techniques in problem solving.
- Introduction to chemistry software programs.
- Application of chemistry software programs.

**PAPER-VI : SYNTHESIS and ANALYSIS OF DRUGS**

**Syllabus:**

**a). Laboratory Synthesis of the following drugs:** Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone,FIuorescien, 4-Aminobenzene sulfonamide, Antipyrine and phenothiazine

**b). Estimation of the following drugs*:*** Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry), colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry),Zn ions in Bactracin Zinc, $Ca^{+2}$ ions in Calcium gluconate injection(complexometry), Riboflavin (UV-Visible Spectrophotometer).

**COURSE OUTCOME:**

- Synthesis Skills: Proficiency in synthesizing pharmaceutical compounds including Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, Fluorescein, 4-Aminobenzene sulfonamide, Antipyrine, and Phenothiazine, with a focus on practical techniques and compound characterization..

- Analytical Techniques Mastery: Competence in various analytical methods such as titrimetry, argentometry, iodometry, colorimetry, complexometry, and UV-Visible spectrophotometry for drug estimation and pharmaceutical analysis.
- Application of Knowledge: Ability to apply synthetic and analytical skills to solve practical problems in drug synthesis, estimation, and quality control within pharmaceutical settings.
- Quality Assurance: Understanding the importance of quality assurance and adherence to standard practices in pharmaceutical synthesis and analysis.
- Career Readiness: Preparation for careers in pharmaceutical research, development, quality control, and regulatory compliance through hands-on experience and theoretical understanding.

**LEARNING OUTCOME:**

- Laboratory synthesis of medicinally important molecules.
- Estimation of purity of different drugs using titremetry, complexometry, iodometry ..etc available in the market and raising the concerns if any.

# M.Sc. CHEMISTRY

## PHYSICAL CHEMISTRY SPECIALISATION
## SYLLABUS OF III & IV SEMESTERS
## *REVISED AS PER NEW (CB) SYLLABUS*

## FOR STUDENTS ADMITTED FROM THE YEAR 2016 ONWARDS

# M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

## Syllabus for III and IV Semesters

**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

***[Under Restructured CBCS Scheme]***

***Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits***

**(Approved in the P.G. BOS meeting held on 01-07-2017)**

## Semester - III (Physical Chemistry)

## *[Under CBCS Scheme]*

**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

| | Hrs/week | Internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH(PC)301T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)302T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)303T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)304T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)351P (LAB-I) | 9 | | | 100 marks | 4 |
| CH(PC)352P (LAB-II) | 9 | | | 100 marks | 4 |
| **Total** | | | | **600 marks** | **24** |

## Semester - IV (Physical Chemistry)

| | Hrs/week | Internal assessment | Semester exam | Total | Credits |
|---|---|---|---|---|---|
| CH(PC)401T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)402T (core) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)403T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)404T (Elective) | 4 | 20 marks | 80 marks | 100 marks | 4 |
| CH(PC)451P (LAB-I) | 9 | | | 100 marks | 4 |
| CH(PC)452P (LAB-II) | 9 | | | 100 marks | 4 |
| **Total** | | | | **600 marks** | **24** |

**Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits**

**M.Sc. SEMESTER - III**
**PHYSICAL CHEMISTRY SPECIALIZATION**
**(for the batches admitted in academic year 2016 & later under CBCS pattern)**

**PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY**
PC - 09: Applications of Schrödinger equation
PC - 10: Angular momentum & approximate methods
PC - 11: Bonding in molecules
PC - 12: Group theory

**PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS**
PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy & Diffraction techniques
PC- 16 : Lasers in Chemistry

**ELECTIVE 3A**
**PAPER III CH (PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS**
PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

**ELECTIVE–3B**
**Paper-III CH (PC) 303T(CB2): Biopolymer Chemistry**
PC-(CB2)- 5:Bioenergetics and physical properties of biopolymers
PC-(CB2)- 6:Biological membranes and binding of ligands by biopolymers
PC-(CB2) - 7: DNA, genes and cloning
PC-(CB2) - 8: Bioinformatics

**ELECTIVE–4A**
**PAPER-IV CH(PC) 304T(CB3): Polymer Chemistry**
PC-(CB3)-9: Polymerization and Kinetics of polymerization
PC-(CB3)-10: Structure and properties of polymers
PC-(CB3)-11: Processing of Polymers
PC-(CB3)-12: Functional polymers

**ELECTIVE –4B**
**Paper IV CH(PC) 304T(CB4): Environmental Chemistry**
PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

**LABORATORY COURSES**

**Paper-V CH (PC) 351 P**: **Chemical Kinetics**
**Paper-VI CH(PC) 352P: Instrumentation**

**M.Sc. SEMESTER - IV**
**PHYSICAL CHEMISTRY SPECIALIZATION**
**(for the batches admitted in the academic year 2016 and later under CBCS pattern)**

**PAPER-1 CH(PC) 401T(CB1): Thermodynamics, Chemical Kinetics and Electrochemistry**
PC- 17.Statistical Thermodynamics
PC- 18. Non-equilibrium Thermodynamics
PC- 19. Chemical Kinetics-II
PC- 20. Electrochemistry –II

**PAPER-II CH(PC) 402T: Supramolecular chemistry, Photo Chemistry and Computational chemistry**
PC-21 : Supramolecular Chemistry
PC-22 : Photochemistry-II
PC-23 : Computational Chemistry
PC-24: Theoretical treatment of bio polymers

**ELECTIVE–3A**
**PAPER-III CH(PC) 403 T(CB1) : Catalysis**
PC-(CB1)-17: Homogeneous catalysis
PC-(CB1)-18: Surface Chemistry and Micellar catalysis
PC-(CB1)-19: Heterogeneous catalysis
PC-(CB1)-20: Phase transfer , Anchored and Photo catalysis

**ELECTIVE–3B**
**Paper IV CH(PC) 403 T(CB2) : Dynamics of chemical reactions and Sensors**
PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23:Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

**ELECTIVE –4A (ID PAPER)**
**PAPER-IV CH(PC) – 404T(CB3) : Computational Chemistry and It's Applications**
PC(CB3)-25: Computational Chemistry – I
PC(CB3)-26: Computational Chemistry – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

**ELECTIVE–4B (ID PAPER)**
**PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry**
PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources:
PC(CB4)- 32 Engineering Materials.

**ELECTIVE–4C (ID PAPER)**
**PAPER-IV CH(PC) 405T(CB5): Sugar Chemistry and Sugar Technology**
PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar and Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

**LABORATORY COURSES**
Paper-V CH (PC) 451P: Chemical Kinetics
Paper-VI CH (PC) 452P: Instrumentation

# M.Sc. SEMESTER - III
# PHYSICAL CHEMISTRY Specialization
**(for the batches admitted in academic year 2016 and later under CBCS pattern)**

## PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

PC -09: Applications of Schrödinger equation
PC -10: Angular momentum and approximate methods
PC -11: Bonding in molecules
PC -12: Group theory

**Learning Objectives:**

- Analyze systems with discontinuous potential fields and quantum tunneling.
- Understand the harmonic oscillator and rigid rotator models.
- Study the hydrogen atom, including wave functions, energies, and probability calculations.
- Learn about atomic and molecular term symbols and the Zeeman effect.
- Understand angular momentum operators, electron spin, and the Pauli principles.
- Learn the Born-Oppenheimer approximation and hybridization concepts.
- Study semiempirical MO methods, Huckel theory, and approximate quantum methods.
- Explore multi-electron atoms, the Hartree-Fock method, and Slater determinants.
- Understand symmetry operations, point groups, and matrix representations.
- Differentiate reducible and irreducible representations and construct character tables.
- Apply group theory in quantum mechanics to analyze wave functions and symmetries.
- Explore vibrational symmetries and predict IR and Raman activity.

**Course Outcomes:**

- Describe potential barriers and quantum mechanical tunneling with examples.
- Solve wave functions and energy levels for harmonic oscillators and rigid rotators.
- Analyze hydrogen atom wave functions, energies, and orthonormal properties.
- Interpret atomic and molecular term symbols and explain the Zeeman effect.
- Define and solve eigenvalue problems for angular momentum operators.
- Apply the Born-Oppenheimer approximation and hybridization in molecular systems.
- Perform Huckel theory calculations and understand approximate methods in quantum mechanics.
- Analyze multi-electron atoms using the Hartree-Fock method and Slater determinants.
- Describe and represent symmetry operations using matrices.
- Generate and interpret character tables for point groups.
- Apply group theory to quantum mechanics, using wave functions and projection operators.
- Analyze molecular vibrations and predict spectroscopic activities

### PC–09: Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - $\alpha$-particle emission, inversion of $NH_3$, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

**PC–10: Angular momentum and approximate methods** (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of $L^2$ and $L_z$ and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Constuction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate ). Wave function and energy corrections. Application of perturbation theory to the helium atom.
Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals ( STOs ).

**PC–11: Bonding in molecules** (15 hrs)

Born-Oppenheimer approximation. MO theory of $H_2^+$ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and enegy diagram. MO theory of $H_2$ molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of $H_2O$. Symmetry-adapted linear combinations. MOs of $H_2O$.

Concept of hybridization – sp, $sp^2$, and $sp^3$ hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. $\pi$–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to extended Huckle Theory, extension of the Huckle's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

**PC–12: Group theory** (15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required ) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for $C_{2h}$, $C_{2v}$ and $C_{3v}$ groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

**Books suggested**:


1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
9. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000).
10. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).


## PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS

PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR, NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy and Diffraction techniques
PC- 16 : lasers in Chemistry

**Learning Objectives:**

- Understand the interaction of electromagnetic radiation with matter, including absorption, emission, selection rules, and factors affecting spectral line width and intensity.
- Learn about infrared and Raman spectroscopy, including principles, selection rules, instrumentation, and applications in structure determination and phase transitions.
- Understand the principles of NMR spectroscopy, including spin-spin splitting, Larmor frequency, and instrumentation for both CW and FT techniques.
- Learn about two-dimensional NMR, nuclear quadrupole resonance, and Mossbauer spectroscopy, including their principles, spectral analysis, and applications.
- Understand the fundamental principles and experimental methods of X-ray fluorescence, analyze the K-emission spectrum of tin and L-emission spectrum of gold, and learn about absorption techniques in X-ray spectroscopy, including AEFS and EXAFS spectra.
- Comprehend the Bragg condition, Miller indices, d-spacing formula, lattice planes, and familiarize with X-ray diffraction methods, including the Laue and Debye-Scherrer methods, and procedures in X-ray structure analysis.

- Learn to index reflections and identify unit cells from diffraction patterns, understand the structure factor, principles of electron diffraction, and apply the Wierl equation to elucidate the structure of simple gas-phase molecules.
- Understand stimulated emission and coherent light production, describe absorption, spontaneous emission, and population inversion, and differentiate between three-level and four-level laser systems, including the role of pumping.
- Define laser light characteristics such as coherence, monochromaticity, directionality, and intensity, discuss laser pulse production methods like Q-switching and mode-locking, and analyze pulse characteristics like duration and peak power.
- Classify different types of lasers based on operational principles and materials, explore practical applications for each type, and understand laser applications in femtochemistry, pump-probe techniques, time-resolved spectroscopy, and molecular dynamics, as well as their role in spectroscopic techniques like two-photon, fluorescence, and Raman spectroscopy.

**Course Outcomes:**

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

- Gain proficiency in analyzing spectral lines, understanding the principles of induced absorption and emission, and applying selection rules to molecular spectra.
- Develop skills in using infrared and Raman spectroscopy for vibrational-rotational analysis of molecules and interpreting spectral data for structural and phase transition studies.
- Gain proficiency in performing and interpreting NMR spectroscopy, including 2D techniques like COSY and NOESY for mixture analysis and structural determination.
- Develop skills in understanding NQR and Mossbauer spectroscopy, analyzing quadrupolar transitions, and interpreting Mossbauer spectra for different iron compounds.
- Demonstrate knowledge of the principles and experimental setup of XRF, and analyze K-emission and L-emission spectra of elements, applying X-ray absorption techniques to investigate material properties and interpret AEFS and EXAFS spectra.
- Apply the Bragg condition, calculate Miller indices and d-spacing, conduct experiments using Laue and Debye-Scherrer methods, index reflections in diffraction patterns, and identify unit cells from systematic absences.
- Describe and present examples of X-ray structure analyses, calculate and interpret the structure factor, explain principles of scattering intensity and angle, and apply the Wierl equation to elucidate the structure of simple gas-phase molecules using electron diffraction data.
- Students will grasp the fundamental principles of laser operation, including stimulated emission, population inversion, and laser cavity design, and will analyze the characteristics of laser light, such as coherence, monochromaticity, and intensity, understanding their practical significance.
- They will learn techniques for generating laser pulses, like Q-switching and mode-locking, differentiate between types of lasers (solid-state, gas, chemical, excimer), and understand their operational principles and practical applications.

- They will explore laser applications in chemistry, such as femtochemistry and time-resolved spectroscopy, and understand their role in molecular dynamics and chemical processes, as well as in spectroscopic techniques like two-photon, fluorescence, and Raman spectroscopy, critically evaluating laser technologies in various contexts.

**PC-13: Physical principles of spectroscopy and Vibrational spectroscopy:** **(**15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral lines.

Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.
Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Strucure determination of $XY_4$ molecules, Phase transitions.

**PC-14: NMR, NQR and Mossbaur Specroscopy.** ( 15hrs)

Prnciple of nmr. Derivation of $h\nu = g\beta H$. Larmor precessional frequency- spin-spin splitting (AX) - Qantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy:
Principles of 2D nmr-Graphical representation of 2D nmr specra – Homonuclear $^1H$ J, $\delta$ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional $^1H$, $^1H$ shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOE). wo dimensional nuclear overhauser spectroscopy (NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – $^{57}Fe$ – Mossbauer spectra of $Fe^{2+}$ and $Fe^{3+}$ (paramagnetic) and $Fe^{3+}$ (magnetic) compounds.

**PC-15: X-ray Spectroscopy and Diffraction techniques:** (15 hrs)

X-ray fluorescence (XRF): Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

**PC-16:Lasers in Chemistry:** (15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.

Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

**Books suggested:**


1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
11. NMR basic principles - Atta-ur-Rahman, Springer.
12. Two-dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Wiley-VCH
13. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
14. Physical Chemistry, Ira N. Levine, McGraw Hill
15. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
16. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
17. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
18. Molecular structure and Spectroscopy, G. Aruldas, Eastern Economic Edn.

**ELECTIVE 3A**

**PAPER III CH(PC) 303T(CB1): APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS**

PC(CB1)-1: Applied kinetics
PC(CB1)-2: Applied Electrochemistry
PC(CB1)-3: Types of materials, conducting organics and NLO materials
PC(CB1)-4: Radiation effects

**Objectives:**

- Understand the fundamental principles of chemical reaction kinetics and its relevance to reactor design.
- Utilize reaction rate laws to describe reaction rates and predict reactor behavior.
- Identify and assess parameters influencing chemical reactor performance, considering design and operational factors.
- Comprehend energy density, power density, and their practical implications in diverse applications.
- Evaluate primary ($Zn/MnO_2$, lead-acid, Ni-Cd) and secondary batteries (lithium cells, lithium-thionyl chloride cells, lithium-ion batteries) for comparative performance.
- Study chemistry and operational principles of fuel cells, including types like $H_2/O_2$ and methanol/$O_2$ fuel cells.
- Classify materials into metals, ceramics, polymers, composites, semiconductors, and biomaterials based on properties and applications.
- Study glass formers, modifiers, and their diverse industrial applications within the glassy state.
- Explore ceramic materials, understanding their crystal structures and structural classifications in various applications.
- Understand radiation's biological impacts, covering acute and chronic effects and influencing factors on organisms.
- Study high-energy radiation types (cosmic rays, gamma rays) and particles (alpha, beta), assessing their biological implications.
- Explore radiation shielding materials and techniques for protection in medical, industrial, and environmental scenarios.

**Outcomes:**

- Explain fundamental principles of reaction kinetics and apply rate laws to determine reaction rates in chemical systems.
- Identify and evaluate key parameters influencing reactor performance, including temperature, pressure, and catalyst properties.
- Assess battery performance by comparing energy density, power density, and Ragone plot data across different battery types.
- Explore hydrogen/oxygen and methanol/oxygen fuel cell operations, detailing their chemistry, advantages, limitations, and efficiency factors.
- Investigate semiconductor-based photovoltaic cells, outlining their materials, operational principles, and efficiency in converting solar energy into electricity.
- Classify materials by categories and compare properties and applications.

- Analyze glassy materials' properties, roles of formers/modifiers, and suitability for applications.
- Discuss properties of conducting organics like fullerenes and doped fullerides for electronics and superconductivity.
- Evaluate radiation hazards to propose protective measures against various exposures effectively.
- Analyze radiation-induced chemical reactions in biological systems to understand the generation and implications of reactive species.
- Apply dosimetry techniques to accurately measure radiation doses and ensure safety in diverse environments.

**PC(CB1)-1:Applied kinetics** (15 hrs)

Kinetics and chemical reaction engineering. Reactor design: Basic objectives in design of a reactor. Parameters affecting the reactor performance. Balance equations for reactor design. Single ideal reactor models.

Batch reactors (BR): General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.

Continuous stirred-tank reactors (CSTR): General features. Design equations for a CSTR. Material and energy balances. Constant-density system. Steady-state operation at specified temperature. Damkohler number – numerical problems.

Plug-flow reactors (PFR): General features. Design equations for a PFR. Material and energy balances. Constant-density system.

Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

**PC(CB1)-2:Applied Electrochemistry** (15 hrs)

Batteries: Battery parameters. Energy density power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. $Zn/MnO_2$, lead-acid and Ni-Cd batteries and Lthium cells; Lithium-thionylchloride cell and lithium-ion battery.
Fuel cells: General Chemistry of Fuel cells. Types of fuel cells: $H_2/O_2$ and methanol/$O_2$ fuel cells. Use of porous electrodes in fuel cells. Advantages, limitations and efficiency of fuel cells.

Photovoltaic cells: Semiconductor based photoelctrochemical cells. Electrochemical energy from solar energy.

Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films.

Electroplating: Technical importance. Mechanism of electroplating. Alkaline and acid plating of copper, nickel.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

**PC(CB1)-3:Types of materials, Conducting Organics and NLO materials** (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications
Ceramics – criteria for determining the crystal structure of ceramic materials – examples.
Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and gels (Zeolite synthesis), crystallization from melts: Czochralski method, Kyropolous method; vapour phase transport method, modification of existing structure by ion-exchange and interaction reactions.

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour. Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.
Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

**PC(CB1)-4: Radiation effects** 15hrs

*Radiation hazards and safety*: Radiation effects. High-energy radiation and high-energy particles – types and sources. Radiation protecting materials.
Radiation chemistry of liquid water. Chemical yields. Dosimetry. Fricke dosimeter and thiocyanate dosimeter. Effect of radiation on DNA. Direct and indirect effects. Reaction of OH radicals with DNA constituents. General mechanism of strand break formation in DNA by OH radicals.

*Radioactive wastemanagement*: Introduction, Classification of radioactive waste, Treatment of Radioactive waste: Radioactive waste disposal.

*Applications of radioisotopes in nuclear medicine and pharmaceuticals*: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization.

**Books suggested:**

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall (page-114)
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
7. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi
8. Electrochemistry – B K Sharma

9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
11. Solid state chemistry and applications. A.R.West, John Wiley & Sons
12. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press
13. Principles of the Solid State, H. V. Keer, New Age International
14. Material Science and Engineering – An Introduction, William D. Callister, Jr., Wiley & Sons
15. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall
16. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
17. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
18. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).
19. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).
20. Nuclear and Radiochemistry G. Friedelarder, J. W. Kennedy, E.. S. Macias, J. M. Miller John Wiley (1981).
21. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)
22. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)
23. Fundamental of Radiochemistry, D.D.Sood, A.V.R.Reddy, N.Ramamoorthy, IANCAs , Mumbai, 4th Edition

**ELECTIVE –3B**

**Paper III CH(PC) 303T(CB2) : BIOPOLYMER CHEMISTRY**

PC(CB2)-5: Bioenergetics & physical properties of biopolymers
PC(CB2)-6: Biological membranes & binding of ligands by biopolymers
PC(CB2)-7: DNA, genes and cloning
PC(CB2)-8: Bioinformatics

**Learning Objectives:**

- Understand ATP's role as the energy currency, coupled reactions, glycolysis, biological redox reactions, and ATP synthesis in mitochondria via the chemiosmotic theory.
- Learn the principles and applications of viscometry, sedimentation, and electrophoresis in studying molecular weights and biopolymer analysis.
- Understand cell membrane structure and function, including equilibria, thermodynamics, osmotic pressure, membrane potentials, and transport mechanisms.
- Explore ion transport, nerve cell action potentials, signal transduction, ligand binding, allosteric interactions, and the Bohr effect in oxygen and $CO_2$ transport.
- Understand the Watson-Crick model of DNA, types of DNA and RNA, and the secondary structure of t-RNA, along with basic principles of gene expression, transcription, translation, and DNA sequencing.

- Explore biotechnology and recombinant DNA technology, including molecular cloning, restriction endonucleases, recombinant DNA construction, DNA hybridization, and DNA fingerprinting technology.
- Understand the use of informatics and computers in biology, including homology and statistical analysis of sequence alignment, and explore general and organism-specific databases for comparative genomics.
- Learn about protein structures at various levels and familiarize with structure databases and homology modeling techniques.

**Course Outcomes:**

- Gain a comprehensive understanding of bioenergetics, including ATP hydrolysis, coupled reactions, and mitochondrial ATP synthesis, along with practical applications of viscometry, sedimentation, and electrophoresis.
- Develop skills to analyze molecular weights, ligand-DNA interactions, and biopolymer properties using advanced biophysical techniques.
- Achieve a deep understanding of cell membrane dynamics, including transport mechanisms, membrane potentials, and signal transduction processes.
- Develop the ability to analyze ligand binding, allosteric interactions, and physiological effects such as the Bohr effect on oxygen and $CO_2$ transport.
- Gain a comprehensive understanding of DNA and RNA structures, gene expression, and the principles of transcription, translation, and DNA sequencing.
- Acquire practical knowledge in biotechnology techniques, including recombinant DNA technology, molecular cloning, and DNA fingerprinting.
- Develop proficiency in using bioinformatics tools and databases for comparative genomics and sequence alignment.
- Gain a thorough understanding of protein structures and acquire skills in homology modeling and utilizing structure databases.



**PC(CB2)-5: Bioenergetics and physical properties of biopolymers** (15 hrs)

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of $H^+$ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

Viscometry: Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers.Light scattering method.

Sedimentation: Sedimentation velocity. Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.

Electrophoresis : principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

**PC(CB2)-6: Biological membranes and binding of ligands by biopolymers** (15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport.

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.
Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of $H^+$ and $CO_2$ . Bohr effect.

**PC(CB2)-7: DNA, genes and cloning** (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA

Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method. Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

**PC(CB2)-8: Bioinformatics** (15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB -
Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures.

Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

**Books suggested:**

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry: Principles and Applications, David Sheehan, John Wiley

4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics, A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxevanis and B. F. Francis Wiley Publishers

**ELECTIVE 4A**

**Paper IV CH(PC) 304T(CB3) :POLYMER CHEMISTRY**

PC(CB3)-9: Polymerization and Kinetics of polymerization
PC(CB3)-10: Structure and properties of polymers
PC(CB3)-11: Processing of Polymers
PC(CB3)-12: Functional polymers

**Learning Objectives:**

- Classify polymers by chemical structure, properties, and industrial applications.
- Study polymerization methods: free radical, cationic, anionic, coordination, and stepwise, emphasizing mechanisms and kinetics.
- Analyze free radical polymerization kinetics, covering degree of polymerization, chain length, transfer coefficients, and the Trommsdorff effect.
- Comprehend polymer dissolution, including thermodynamic aspects like entropy and free energy of mixing in solutions.
- Explore polymer chain conformations, including the freely jointed chain model and interactions at short and long ranges.
- Understand Flory-Huggins theory, its application to dilute polymer solutions, and its extension to polymer mixtures via Flory-Krigbaum theory.
- Understand polymers' widespread applications across industries such as automotive, construction, packaging, electronics, healthcare, and textiles.
- Examine the role of polymer additives like fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, and flame retardants in enhancing polymer properties.
- Explore diverse polymer processing techniques including coating, extrusion, molding, casting, and fiber reinforced plastics, analyzing their applications and material properties.
- Explore Smart Materials: Understand principles and applications in sensing devices and communication networks, focusing on responsiveness to stimuli.
- Study Electrically Conducting Polymers: Introduce principles and explore applications in electronics, sensors, and actuators with polymers like polyanilines and polypyrrole.
- Examine Photoconductive Polymers: Explore optoelectronic device applications, emphasizing light-to-electrical signal conversion capabilities.

**Course Outcomes:**

- Classify polymers by molecular structure, properties, and applications, comparing synthesis methods and properties across polymer types.

- Analyze polymerization kinetics across techniques like free radical, cationic, anionic, and coordination, examining mechanisms and reaction dynamics.
- Evaluate how pressure, temperature, and other variables influence chain polymerization kinetics and outcomes effectively.
- Apply thermodynamics to analyze polymer dissolution processes, including entropy and free energy changes in solutions.
- Analyze polymer chain conformations in solution using theoretical models and examine polymer-solvent interactions.
- Evaluate the Flory-Huggins theory's application in predicting polymer-solvent interactions in both dilute and concentrated solutions.
- Apply polymer knowledge to select appropriate materials for specific industrial applications based on their properties and performance.
- Evaluate the influence of polymer additives on material properties and performance, choosing additives suitable for desired applications.
- Demonstrate proficiency in polymer processing techniques like coating, extrusion, molding, casting, and fiber reinforcement to produce high-quality polymer-based products.
- Innovate with smart materials for responsive sensing devices and networks that adapt to stimuli.
- Explore electrically conducting polymers' roles in electronics, sensors, and advanced tech.
- Apply polymer membranes for efficient liquid and gas separation in industries.
- Create biocompatible polymer-based biomedical devices like artificial organs and drug delivery systems.

**PC(CB3)-9: Polymerization and Kinetics of polymerization** (15 hrs)

Classification of polymers. Types of polymerization.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization.

copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization-Bulk, solution, suspension and emulsion polymerizations.

**PC(CB3)-10: Structure and properties of polymers** (15 hrs)

Polymer solutions:

The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers:

The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.

The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of Tm. Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization.

The glassy state – glass transition temperature Tg of polymers. Factors influencing Tg. Glass transition temperature and melting point.

Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC.

**PC(CB3)-11: Processing of Polymers** (15hrs)

General applications of Polymers. Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardents.

Processing techniques of polymers - one dimensional coating -Adhesives, Lamination; extrusion-calendering and thermoforming ; Molding of Polymers- Process, advantages and limitations of Compression molding, Injection Molding, Extrusion Molding, Blow Molding.

Casting - Types, Vacuum Casting, Potting, Encapsulation, Film Casting,.

Fibre Reinforced Plastics- preparation and properties. Synthetic Fibres- Rayons, (Nitro cellular, Cupammonium, Diacetate, Viscose), Nylons, Dacron.

Processing of fiber reinforced Composites- Pultrusion technique, prepreg production processes, filament winding.

**PC(CB3)-12: Functional polymers** (15hrs)

Smart materials – Their uses in sensing devices and in communication networks.

Electrically conducting polymers- Introduction, basic principles and their applications. Brief description of polyanilines, polypyrrole, polyacetylene and polythiophene.

Photoconductive polymers, Liquid crystal polymers – smectic, nematic and cholesteric structures, Ionic exchange polymers- Cationic and anionic exchange polymers and their uses.

Biodegradable polymers- Definition, classification, applications. Brief description of polyhydroxyalkanoates, polycaprolactone, polyacetic acid and polyvinylalcohol.

Polymers in Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis.

Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.

**Books suggested:**

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall

4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional
5. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers
6. Polymer Chemistry, B. Vollmert, Springer publishers
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
8. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar, S. Chand publishers

**ELECTIVE 4B**

**Paper IV CH(PC) 304T(CB4) : ENVIRONMENTAL CHEMISTRY**

PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

**Learning Objectives:**

- Understand the typical composition of unpolluted dry air and identify major air pollutants, their sources, effects, and control methods, including carbon monoxide, nitrogen oxides, sulfur oxides, particulate matter, and hydrocarbons.
- Learn about environmental issues like the greenhouse effect, ozone depletion, and notable disasters such as the Bhopal Gas Tragedy and Seveso Disaster, including their causes, consequences, and abatement strategies.
- Understand the types, sources, and effects of water pollutants, including persistent pollutants, biomagnification, eutrophication, and bacteriological contamination.
- Learn about the impact of dissolved oxygen depletion, biological and chemical oxygen demand, toxic effects of nitrates, nitrites, and nitrosoamines, and methods for treating drinking water supplies.
- Understand essential and toxic elements in nature, mechanisms of metal ion toxicity, and their effects on biological systems, along with concepts of speciation, biomethylation, and biomagnification.
- Learn about the sources, speciation, and biochemical effects of mercury, arsenic, lead, cadmium, and radiochemical pollution, including case studies like Minamata Bay and the Chernobyl disaster.
- Understand air quality standards, sampling methods, and analysis techniques for various pollutants, including particulates, $SO_2$, $H_2S$, NO-NOx, CO, hydrocarbons, and ozone.
- Learn water sampling, preservation, and analysis methods, including physical and chemical analysis of anions, and determination of DO, BOD, COD, and TOC in water.

**Course Outcomes:**

- Gain a thorough understanding of the composition of unpolluted air, major air pollutants, their impacts, and control measures.
- Develop awareness of environmental issues such as the greenhouse effect, ozone depletion, and industrial disasters, along with strategies for their mitigation.
- Gain a comprehensive understanding of water pollution, including types of pollutants, their sources, and ecological and health impacts.
- Develop knowledge of water quality indicators and acquire skills in water treatment methods to ensure safe drinking water supplies.
- Gain knowledge of the mechanisms of metal ion toxicity, their effects on biological systems, and key environmental concepts like speciation and biomagnification.
- Understand the sources, environmental pathways, and biochemical impacts of pollutants such as mercury, arsenic, lead, cadmium, and radioactive materials, including case studies and mitigation strategies.
- Develop proficiency in sampling and analyzing air pollutants using various spectrometric and chromatographic techniques to ensure compliance with air quality standards.
- Gain skills in water sampling, preservation, and comprehensive analysis of physical and chemical parameters to assess and maintain water quality.



**PC(CB4)-13: Pollution in Atmosphere**

Typical Composition of Unpolluted Dry Air - Major Air Pollutants: Carbon Monoxide, Nitrogen Oxides, Sulphur Oxides, Particulate Matter, Hydrocarbons, Chloroflurocarbons.

Carbon Monoxide: Sources and Sinks, Concentration Profile, Effects on Human Health, Control of CO Emissions.

Nitrogen Oxides ($NO_x$): Reactions Leading to Formation of $NO_x$, Sources and Sinks, Concentration Profile, Harmful Effects of $NO_x$ on Human Beings, Plants, Materials and Control of $NO_x$ Emissions.

Sulphur Oxides ($SO_x$): Reactions Leading to Formation of $SO_x$, Sources of $SO_x$. Harmful Effects on Human Beings, Plants and Materials - Control of $SO_x$ Emissions - Acid Rain: Formation and Toxic Environmental Effects.

Particulate Matter: Sources, Inorganic and Organic Particulate Matter - Effects on Human Beings, Materials and Climate - Control of Particulate Emissions.

Hydrocarbons: Sources - Types of Polluting Hydrocarbons - Hydrocarbons and Photochemical Smog Formation - Harmful Effects of Photochemical Smog - Control of Hydrocarbon Emissions.

Green House Effect: Causes, Consequences and Abatement of Green House Effect - Ozone Depletion - Mechanism, Causes, Consequences and Abatement of Ozone Depletion - Bhopal Gas Tragedy and Sevozo Disaster.

**PC(CB4)-14: Pollution in Hydrosphere**

Types of Water Pollutants and their Effects - Sources of Water Pollution: Domestic, Industrial, Agricultural, Soil, Thermal and Radioactive Wastes - Types of Persistent Pollutants - Biomagnification of Persistant Pollutants, Effects of Biomagnified Pollutants on Human Beings (DDT) – Tripolyphosphates: Their Role in Eutrophication of Water Bodies - Ecological Consequences of Eutrophication, Bacteriological Contamination of Water - Dissolved Oxygen in Natural Waters - Depletion of Dissolved Oxygen - Biological Oxygen Demand and Chemical Oxygen Demand as Indicators of Extent of Water Pollution - Nitrates, Nitrites, Nitrosoamines in Water: Their Toxic Effects On Human Beings - Treatment of Drinking Water Supplies.

**PC(CB4)-15: Heavy Metal and Radiochemical Pollution.**

Essential and Toxic Elements in Nature - Mechanism of Metal Ion Toxicity - Effects on Non-Metalloenzymes, Metalloenzymes, Cell Membranes, Nucleic Acids - Concepts of Speciation, Biomethylation and Biomagnification.

Mercury: Sources of Pollution. Speciation and Environmental Forms of Mercury - Biochemical Effects of Different Species of Mercury - Minamata Bay Episode as a Case Study of Mercury Poisoning.

Arsenic: Sources of Pollution - Speciation and Environmental Chemistry of Arsenic - Biochemical Effects of Different Species of Arsenic.

Lead: Sources of Lead Pollution - Speciation and Pathways of Lead in Environment - Biochemical Effects of Lead.

Cadmium: Sources of Pollution – Speciation - Biochemical Effects of Cadmium Poisoning.
Radiochemical Pollution: Sources, Chemical Changes due to Radiation on Water.

Organic Compounds - Harmful Effects of Radioactive Pollutants on Living Organisms - Permissible Limits of Radiation - Control and Disposal of Radioactive Wastes - Chernobyl Disaster.

**PC(CB4)-16: Analysis of Air, Water and Metal Pollutants**

Air Quality Standards - Sampling (Particulates and Gaseous Pollutants) - Analysis of Pollutants: $SO_2$ (Modified West-Gaeke Spectrophotometric Method, Pulsed Fluorescence Spectrometry), $H_2S$ (Spectrophotometry – Ethelyne Blue Method), NO-NOx (Chemiluminescence Technique, Colorimetric Technique- Saltzman Method) – CO (NDIR Spectrometry, GC), Hydrocarbons (Ionization Analysis), Aromatic Hydrocarbons in Automobile Exhausts, Petrol, Air, $O_3$ (Chemiluminiscene and Spectrophotometry) - Particulate Matter Analysis (High Volume Method).

Water Sampling, Preservation and Preconcentration Methods and Physical Analysis - Colour, Odour, Temperature, pH, EC, Redox Potential and Total Dissolved Solids (Turbidimetry). Chemical Analysis of Anions: $CN^-$, $Cl^-$, $F^-$ (Spectrophotometry, Ion Selective Potentiometry and Titrimetry), $NO_2^-$ and $NO_3^-$ (Spectrophotometry), $SO_4^{2-}$, $PO_4^{3-}$, $HCO_3^-$, $CO_3^{2-}$, Hardness of Water (Titrimetry), Ammonical Nitrogen (Spectrophotometry) - Determination of DO, BOD, COD, TOC in Water.

**Books Suggested:**

1. Environmental Chemistry, John. W. Moore and Elizabeth Moore Academic press New York
2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Ed.
3. Environmental Chemistry, 4th ed. A.K. De. New Age International Publishers, 2000
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. 1995
5. Environmental Chemistry, Colin Baird W.H. Freeman and Company New York 1995.

6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers
7. Chemistry of the Environment, II Edn., Thomas G. Spiro William M. Stigliani
8. Fundamental Concepts of Environmental Chemistry, G.S. Sodhi Narosa Publishing House.
9. Environmental Analytical Chemistry, F.W. Fifield, P.J. Haines, Blackie Academic & Professional

## III SEMESTER PRACTICALS

**CH (PC) 351 P: Paper-V (Chemical Kinetics)** **9** hrs/week

**Course Objectives:**

- The learners should be able to validate the conceptual understanding acquired from the theory classes

**Learning Outcomes**: At the end of the course, the learners should be able to:

- **Explain** the principle behind the experiments performed in the laboratory
- **Plan** and **Perform** experiments and **Interpret** experimental results

**Note:** The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

- Study of peroxydisulphate – iodide reaction:
  1. Individual orders of the reactants by initial rate and isolation methods
  2. Effect of temperature on reaction rate
  3. Effect of ionic strength on reaction rate
- Study of peroxydisulphate – iodide clock reaction:
  1. Individual orders of the reactants,
  2. effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions
- Study of acetone – iodine reaction by titrimetry
  1. Order w.r.t. [ iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H+]

**CH (PC) 352: Paper-VI (Instrumentation)** 9 hrs/ week

**Course Objectives:**

- The learners should be able to validate the conceptual understanding acquired from the theory classes

**Learning Outcomes**: At the end of the course, the learners should be able to:

- **Explain** the principle behind the experiments performed in the laboratory
- **Plan** and **Perform** experiments and **Interpret** experimental results
- **Record data and analyze** it obtained from Instrumental operation and experimentation.

**Conductometry:**

- Conductometric titrations:
  1. Mixture of strong and weak bases vs strong acid
  2. Mixture of strong and weak acids vs weak base
  3. Mixture of strong acid, weak acid and $CuSO_4$ vs strong base
  4. Mixture of halides (chloride + iodide) vs $AgNO_3$
  5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid

6. and their mixtures vs strong base
7. Precipitation titration: K2SO4 vs BaCl2

- ♦ Dissociation constants of weak acids
- ♦ Effect of solvent on dissociation constant of a weak acid
- ♦ Verification of Onsager equation
- ♦ Composition of Cu(II) – tartaric acid complex by Job's method

**pH metry:**

- ♦ pH – metric titrations:
  1. Monobasic acids vs strong base
  2. Dibasic acid vs strong base
  3. Tribasic acid vs strong base
  4. Mixture of strong and weak acids vs strong base
- ♦ Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
- ♦ Determination of dissociation constant of acetic acid in DMSO, acetone anddioxane
- ♦ Determination of pKa and pKb of glycine (calculation using a computerprogram)
- ♦ Determination of stability constant of a metal complex

**Suggested books:**

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B. Yadav

## M.Sc. SEMESTER - IV
## PHYSICAL CHEMISTRY SPECIALIZATION
**(For the batches admitted in academic year 2016 and later under CBCS pattern)**

**PAPER I CH(PC)401: <u>Thermodynamics, Chemical kinetics and Electrochemistry</u>**

PC-17 : Statistical Thermodynamics
PC-18 : Non-equilibrium Thermodynamics
PC-19 : Chemical Kinetics-II
PC-20 : Electrochemistry -II

**Objectives:**

- Understand distribution, probability, and the Boltzmann distribution.
- Learn about molecular and canonical partition functions.
- Explore thermodynamic functions, specific heats, and entropy.
- Study Bose-Einstein, Fermi-Dirac, and Maxwell-Boltzmann statistics.
- Understand thermodynamic criteria for non-equilibrium states and entropy production.
- Learn flux-force relations, Onsager reciprocal relations, and microscopic reversibility.
- Apply Onsager relations to electrokinetic phenomena and liquid junction potentials.
- Explore irreversible thermodynamics in biological systems and thermoelectric circuits.
- Identify and analyze factors affecting reaction rates in solution, including concentration, temperature, pressure, solvent properties (dielectric constant, ionic strength), and solvent effects.

- Analyze factors affecting reaction rates in solution, including pressure, diffusion, dielectric constant, and ionic strength.
- Study fast reaction techniques and kinetic methods.
- Understand enzyme kinetics, including Michaelis-Menten mechanisms, kinetic equations, and enzyme-substrate interactions.
- Explore enzyme specificity, pH dependence, and enzyme inhibition.
- Understand the structure and properties of the electrical double layer at electrode-electrolyte interfaces, including models like the Helmholtz-Perrin, Gouy-Chapman, and Stern models.
- Introduce quantum mechanical principles relevant to charge transfer at electrode surfaces, covering tunneling phenomena and their implications.
- Analyze charge transfer reactions at electrode-electrolyte interfaces, deriving the Butler-Volmer equation, exchange current density, overpotential, and Tafel equation under various field approximations.

**Outcomes:**

- Estimate probabilities and derive the Boltzmann distribution.
- Relate partition functions to thermodynamic properties.
- Explain specific heats using Einstein and Debye theories.
- Compare Bose-Einstein, Fermi-Dirac, and Maxwell-Boltzmann statistics.
- Describe entropy production in heat and material flow in irreversible processes.
- Derive and apply linear flux-force relations and Onsager reciprocal relations.
- Analyze electrokinetic phenomena and liquid junction potentials using Onsager relations.
- Apply principles of irreversible thermodynamics to biological systems and thermoelectric effects.
- Describe how pressure, diffusion, and ionic strength influence reaction rates in solution.
- Apply methods for studying fast reactions, including flow, fluorescence, and relaxation techniques.
- Derive and evaluate kinetic parameters for enzyme-catalyzed reactions and understand enzyme-substrate complex models.
- Analyze enzyme specificity, pH effects on enzyme kinetics, and enzyme inhibition mechanisms.
- Analyze the structure and behavior of the electrical double layer using theoretical models, applying insights to interpret electrochemical interface phenomena.
- Utilize quantum mechanical principles to predict charge transfer processes at electrode surfaces, including tunneling effects impacting electrochemical reactions.
- Derive the Butler-Volmer and Tafel equations under various conditions, applying them to calculate and interpret electrochemical reaction rates and overpotentials, facilitating deeper understanding of electrochemical kinetics.

**PC -17: Statistical Thermodynamics** (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory. The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

**PC-18: Non-equilibrium Thermodynamics** (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.

Fluxes and forces. Linear flux-force relations**.** Phenomenonological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations.

Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.

Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.

**PC-19: Chemical kinetics – II:** (15hrs)

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P- jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

**PC –20 : Electrochemistry – II** (15 hrs)

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion.Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion.Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

**Books suggested:**


1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Text book of Biochemistry by Stryer, W.H.Freeman & Co Ltd
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
9. Chemical Kinetics, K. J. Laidler, McGraw Hill
10. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
12. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
13. Physical Organic Chemistry, N. S. Isaacs, ELBS
14. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
15. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
16. Modern Electrochemistry 2B, Bockris & Reddy, Plenum.
17. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi


**PAPER- CH(PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY**

PC-21: Supramolecular Chemistry
PC-22: Photochemistry
PC-23: Computational Chemistry
PC-24: Theoretical treatment of bio polymers

**Objectives:**

- Define and differentiate molecules, supermolecules, and supramolecules, emphasizing their hierarchical structures and interactions in various contexts.
- Examine non-covalent supramolecular interactions including hydrogen bonding, $\pi$-$\pi$ interactions, electrostatic forces, and van der Waals interactions.

- Investigate molecular recognition principles involving shape complementarity, hydrogen bonding, hydrophobic effects, and ion-dipole interactions, essential for designing molecular receptors and ionophores.
- Understand the formation of excimers and exciplexes, PE diagrams, quantum yields, and energy transfer mechanisms, including bimolecular quenching and various energy transfer processes.
- Learn about P-type delayed fluorescence, experimental methods for studying photochemical reactions, and electronic transitions in transition metal complexes.
- Classify and describe biopolymers such as proteins, nucleic acids, polysaccharides, and lipids, emphasizing their structural and functional roles in biology.
- Explore experimental methods to determine biopolymer size and shape, including sedimentation analysis, light scattering techniques, and colligative properties.
- Analyze polypeptide chain conformation and secondary structures like α-helices and β-sheets, and discuss their formation principles and energetic considerations.
- Understand multi-electron atoms, the anti-symmetry principle, Slater determinant, and the Hartree-Fock method, including key concepts like the Fock operator, Coulomb and exchange operators, and Slater-type orbitals.
- Learn about restricted and unrestricted HF calculations, basis sets, and the application of HF methods to simple molecules, as well as an introduction to density functional theory (DFT) and the Kohn-Sham formulation.

**Outcomes:**

- Differentiate between molecules, supermolecules, and supramolecules based on their structural hierarchies and interactions in diverse contexts.
- Analyze supramolecular interactions driven by non-covalent forces like hydrogen bonding and van der Waals interactions, predicting their impacts on materials and biological systems.
- Apply principles of molecular recognition to design and synthesize molecular receptors with tailored binding affinities, demonstrating proficiency in host-guest chemistry and macrocyclic synthesis.
- Gain proficiency in analyzing energy transfer mechanisms, understanding delayed fluorescence, and utilizing experimental techniques to study photochemical reactions.
- Develop skills in identifying electronic transitions in transition metal complexes, exploring ligand field and charge transfer states, and applying knowledge to photoredox reactions and photochemical water cleavage.
- Gain proficiency in applying the Hartree-Fock method to multi-electron atoms and molecules, interpreting results from HF calculations, and understanding theoretical principles like Hund's rules and Koopman's theorem.
- Develop skills in using density functional theory (DFT) to study electronic structures, including an understanding of the Hohenberg-Kohn theorem, Kohn-Sham equations, and exchange-correlation energy.
- Classify biopolymers based on their chemical composition, structure, and biological functions, comparing their properties and roles in biological systems.
- Apply experimental techniques to characterize biopolymers, interpreting data from sedimentation analysis, light scattering, and colligative properties to understand their size and shape.

- Analyze polypeptide chain conformation and configuration using theoretical models and experimental data, calculating size and shape metrics to elucidate polymer behavior and structure.

**PC-21: Supramolecular Chemistry**

*Concepts:* Molecules, super molecules and supramolecules. Nature of Supramolecular interactions. Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles.

Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, calixaranes, and cyclodextrins - their selectivity, macrocyclic, and template effects. Fullerenes as supramolecules.

Threading of a linear molecule through a cyclic molecule –creation of Rotaxanes and Catenanes.

Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Supramolecular catalysis- Crownether supported alkaline earth metal ions as catalysts, cyclodextrins and calixaranes as catalysts in chemical reactions. Transport of ions across membranes by biological molecules.

Molecular electronic devices: Molecular wires, molecular switches and machines.

**PC-22: Photochemistry – II**

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

P-type delayed fluorescence. The experimental study of photochemical reactions: Product analysis, chemical methods in the study of intermediates, spectroscopic methods, ESR and CIDNP, rate coefficients for photochemical processes and identification of excited states.

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $Ru(bpy)_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

**PC-23: Computational treatment of many electron systems** (15 hrs)

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations (no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.

The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on $H_2$. Discussion of results of HF calculations on simple molecules – $H_2O$ and $NH_3$. Introduction to configuration interaction.

Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

**PC-24: Theoretical treatment of biopolymers** (15 hrs)

Types of biopolymers. Methods of determining Size and shape of biopolymers - mean molecular masses, colligative properties, sedimentation, viscosity, light scattering methods.

Chain conformation and configuration of poly peptides. Random coils and measures of size – contour length, rms separation, radius of gyration, constrained chains.

Secondary structures of proteins- helices and sheets: The Corey-Pauling rules. Conformational energy of a polypeptide- bonding, nonbonding potentials, electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds. Principles of molecular mechanics to calculate potential energy of a polypeptide. Ramachandran plots of α-helix and β-sheet.

Conformational entropy. Introductory treatment of the protein folding problem.

**Books suggested:**


1) J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.
3) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons.
4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
6) Quantum Chemistry, I. N. Levine, Prentice Hall
7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
9) Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers
11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.
13) Physical Chemistry, P. W. Atkins, Oxford Unibersity Press.
14) Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
17) Physical Biochemistry: Principles and Applications, David Sheehan, John Wiley
18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books


**ELECTIVE –3A:**

**PAPER III CH(PC)- 403T(CB1): CATALYSIS**

PC(CB1)-17: Homogeneous catalysis

PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer, Anchored & Photo catalysis

**Learning Objectives:**

- Introduce fundamental concepts of catalysis, emphasizing catalysts' role in accelerating reactions without being consumed.
- Classify and explore various types of catalysis (homogeneous, heterogeneous, enzyme, metal-ion) to understand mechanisms and applications in industrial and environmental contexts.
- Describe catalyst characteristics (selectivity, activity, stability) and examine the role of supports and promoters in enhancing catalytic performance across different applications.
- Understand the principles of surface tension, curved interfaces, the Laplace equation, capillary action, and the thermodynamics of surface layers including the Gibbs isotherm, as well as the types and factors affecting adsorption, and the thermodynamics and determination of heats and entropies of adsorption.
- Differentiate between surface and bulk structures, comprehend adsorbate-induced restructuring of surfaces, thermal activation of bond breaking, co-adsorption, and the kinetics of chemisorption, and explore the properties and reactions on monometallic and bimetallic surfaces, including experimental techniques for monolayer films.
- Learn about micellization, micellar interactions, and structures, understand critical micellar concentration (CMC) and factors affecting it, thermodynamics of micellization, and applications in phase separation, solubilization, microemulsions, and reactions assisted by micelles, with examples of micelle-catalyzed reactions.
- Identify and classify different types of catalysts, including metals, semiconductors, and nanomaterials, and learn methods for preparing these catalysts.
- Understand key steps and mechanisms in heterogeneous catalysis, analyze kinetics and thermodynamics of catalyzed reactions, and distinguish between structure-sensitive and structure-insensitive catalysts.
- Learn techniques for determining surface area and pore size distribution (e.g., BET, BJH methods), measure surface acidity, and utilize surface characterization techniques (e.g., XRD, TEM, XPS) with comprehensive knowledge in heterogeneous catalysis for industrial and environmental applications.
- Understand the principles and classification of phase-transfer catalysis (PTC), the role of water, factors influencing reaction rates, and inverse phase-transfer catalysis, including mechanisms of nucleophilic displacement reactions.
- Learn about crown ethers as PTCs in reactions with alkyl halides and permanganate oxidation of alkenes and phenols, and explore anchored catalysis with organic polymers, inorganic oxides, and clays, focusing on montmorillonite catalysts and their applications in hydrogenation.
- Comprehend the photocatalytic effect and metal semiconductor systems, including the influence of metal loading and semiconductor properties, and explore applications of photocatalysis in water splitting, pollutant removal, and organic compound oxidation and reduction.

**Course Outcomes:**

- Classify and compare types of catalysis, detailing their mechanisms, advantages, and limitations across different applications.
- Analyze catalyst characteristics and assess their activity using experimental data and theoretical models to predict reaction rates under varying conditions.
- Apply equilibrium and kinetic approaches to analyze catalytic reactions, understanding how catalysts influence reaction pathways and selectivity.
- Demonstrate an understanding of surface tension, curved interfaces, the Laplace equation, capillary action, and the thermodynamics of surface layers including the Gibbs isotherm, as well as types, factors, and thermodynamics of adsorption, and methods for determining heats and entropies of adsorption.
- Analyze the differences between surface and bulk structures, understand adsorbate-induced restructuring, thermal activation of bond breaking, co-adsorption, and the kinetics of chemisorption, and investigate properties and reactions on monometallic and bimetallic surfaces, using experimental techniques for monolayer films.
- Comprehend micellization, micellar interactions, and structures, understand critical micellar concentration (CMC) and factors affecting it, the thermodynamics of micellization, and apply knowledge of micelles in phase separation, solubilization, microemulsions, and reactions, including examples of micelle-catalyzed reactions.
- Identify and classify various catalysts, including metals, semiconductors, and nanomaterials, and apply different methods for preparing metal and non-metallic catalysts.
- Describe the key steps and mechanisms in heterogeneous catalysis, analyze reaction kinetics and thermodynamics, and determine factors affecting catalytic activity, including distinguishing structure-sensitive and structure-insensitive catalysts.
- Determine surface area using BET and analyze pore volume and size using BJH methods, measure surface acidity, and apply surface characterization techniques like XRD, TEM, and XPS, while understanding the role of catalytic converters and various industrial catalytic processes.
- Demonstrate an understanding of the principles, classification, and role of water in phase-transfer catalysis (PTC), and identify factors influencing the rate of PTC reactions, including inverse phase-transfer catalysis and nucleophilic displacement mechanisms, the role of crown ethers as PTCs in reactions involving alkyl halides and permanganate oxidation of alkenes and phenols.
- Understand the concept of anchored catalysis with examples, focusing on the structure and application of montmorillonite catalysts in hydrogenation.
- Describe the photocatalytic effect, characteristics of metal semiconductor systems, and the influence of metal loading and semiconductor properties, and apply photocatalysis to water splitting, pollutant removal, and organic compound oxidation and reduction.

**PC(CB1)-17: Homogeneous catalysis** ( 15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid-base strength- Bronsted relationships.

Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function(Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

**PC(CB1)-18: Surface Chemistry and Micellar catalysis** (15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.

Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption.

Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.

*Micelles:* Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

**PC(CB1)-19: Heterogeneous catalysis** (15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non- metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts-

Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

**PC(CB1)-20: Phase transfer, Anchored and Photo catalysis** **(**15 hrs)

*Phase-transfer catalysis (PTC):* Principles of phase-transfer catalysis. PTC classification. Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts (PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quartemary ammonium salts and crown ethers.

*Anchored catalysis:* Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

*Photo catalysis:* Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

**Books suggested:**


1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry, M. Satake, Y. Hayashi, Y. Mido, S.A. Iqbal and M.S. Sethi
6. "Physical Organic Chemistry" by L.P. Hammett, chapter 9, McGraw Hill.
7. Chemical Review, **57,** 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed ), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M.Thomas andW.J.Thomas, VCH1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet.
19. Modern methods of Organic Synthesis: Ahluwalia.

**ELECTIVE–3B**

**PAPER IV CH(PC) 403 T(CB2): Dynamics of Chemical Reactions And Sensors**

PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC-(CB2)-23: Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

**Learning Objectives:**

- Understand the Huckel molecular orbital method, advanced PMO and FMO theories, molecular mechanics, and various computational methods, including their scope and limitations.
- Learn about quantitative MO theory, orbital symmetry, and interaction diagrams, along with the MO of simple organic systems, conjugation, hyperconjugation, aromaticity, and VB configuration mixing.
- Understand the theory of isotope effects, solvent effects, and structural effects on reactivity, including LFER, Hammett equation, and solvation measures.
- Explore steric effects on reactivity, conformational barriers, and principles like Winstein-Holness and Curtin-Hammett.
- Understand the concepts of bases, nucleophiles, electrophiles, and catalysts, along with acid-base dissociation, electronic and structural effects, and nucleophilicity scales.
- Explore mechanisms and effects on $S_N1$, $S_N2$, $SR_N1$, electrophilic reactivity, and the dynamics of radical and pericyclic reactions.
- Understand the importance of sensors and biomolecular recognition elements, including artificial materials and electrode modifications, along with various sensor types like fluorescence, conductometric, and voltammetric sensors.
- Explore the principles and applications of advanced sensors, including those for neurotransmitters, electrochemical impedance, surface plasmon resonance, and fiber optic sensors, particularly in food safety and biomedical diagnostics.

**Course Outcomes:**

- Gain proficiency in applying theoretical and computational methods to explain molecular structures and energy levels, particularly using Huckel MO theory.
- Develop the ability to analyze reaction profiles, potential energy diagrams, and the mechanistic significance of thermodynamic parameters in chemical reactions, using concepts like the Arrhenius equation and transition state theory.
- Develop the ability to analyze kinetic isotope effects, solvent-solute interactions, and structural influences on chemical reactivity.
- Gain proficiency in using theoretical models and empirical indexes to study reaction mechanisms, steric effects, and conformational dynamics in organic systems.

- Gain proficiency in analyzing acid-base catalysis, nucleophilic and electrophilic reactivity, and the role of structural and electronic effects in various reaction mechanisms.
- Develop skills in applying theoretical models to study reaction kinetics, solvent effects, and the principles governing radical and pericyclic reactions.
- Gain knowledge of different sensor technologies, their working principles, and their applications in detecting biomolecules and chemical substances.
- Develop skills in utilizing advanced sensors for practical applications in fields such as food safety and biomedical diagnosis, including detecting mycotoxins, adulterants, and cancer markers.

**PC-(CB2)-21: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity** 15 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels .Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters.

**PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects** 15 Hrs

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1, σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

**PC-(CB2)-23: NUCLEOPHILIC, ELECTROPHILIC AND FREE RADICAL REACTIVITY** 15 Hrs

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases.

Nuccleophilicity scales, Nucleofugacity. The α-effect.- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronstéd catalysis. .nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and S2 reactivity based on curve-crossing rnodel. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity. ; Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

**PC-(CB2)-24: Chemical, Electrochemical and Bio Sensors** 15hrs

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bio-luminescence sensors, Fluorescent tag molecules, Applications. Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors, Molecular recognition, Applications. Surface Plasmon resonance-based sensors, Fiber optic sensors, Twodimensional microarray-based sensors, Applications for Food Safety - Mycotoxins, adultrants, Biomedical diagnosis - Cancer markers.

**Books suggested:**

1. Molecular mechanics. By U. Bukert and N.L. Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L. Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M. Lowry, K.C. Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH, Weinhein.
5. Physical Organic chemistry, N.S.Isaaçs
6. Suprarnolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack HineLaboratory course
9.Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
10.Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
11. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.

**ELECTIVE –4A (ID PAPER)**

**PAPER III CH(PC)- 403T(CB3): MOLECULAR MODELING AND IT'S APPLICATIONS**

PC(CB3)-25: Molecular Modeling – I
PC(CB3)-26: Molecular Modeling – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

**Learning Objectives:**

- Understand the basics of molecular modeling, including single molecule calculations, assemblies, reactions, and coordinate systems like Cartesian and Internal Coordinates.
- Learn about potential energy surfaces, conformational search, and molecular mechanics features, including bonded and non-bonded interactions.
- Understand the force field equation in energy minimization, derivative minimization methods, and types of energy minimization methods such as Steepest Descent and Conjugate Gradient.
- Learn about molecular dynamics, Monte-Carlo methods, and the differences between them, including basic elements and applications in simulations.
- Understand the concepts of Structure Activity Relationship (SAR) and Quantitative Structure Activity Relationship (QSAR), and the physicochemical parameters influencing these relationships.
- Learn about molecular descriptor analysis, regression analysis for QSAR equations, and the differences between 2D and 3D QSAR techniques.
- Understand database similarity searches, pair-wise alignment methods (global and local), multiple sequence alignment, and the process of homology modeling.
- Learn techniques for model evaluation, active site identification, docking algorithms, molecular interactions, scoring functions, and virtual screening, including de novo ligand design.

**Course Outcomes:**

- Gain proficiency in performing molecular modeling and conformational analysis using different coordinate systems and understanding potential energy surfaces.
- Develop skills in applying molecular mechanics to analyze bonded and non-bonded interactions, including electrostatic, Van-der Waals, and hydrogen **bonding interactions.**
- Gain proficiency in applying energy minimization techniques and geometry optimization procedures in molecular modeling.
- Develop skills in performing molecular dynamics and Monte-Carlo simulations to analyze molecular behavior and properties.
- Develop skills in distinguishing between SAR and QSAR, analyzing electronic effects, hydrophobicity, and steric factors using various models and descriptors.
- Gain proficiency in performing regression analysis and applying 3D QSAR techniques like CoMFA and CoMSIA to study and predict molecular activity.
- Gain proficiency in performing sequence alignments, homology modeling, and evaluating models using various tools and techniques.
- Develop skills in identifying active sites, conducting docking studies, understanding scoring functions, and applying virtual screening methods to design and evaluate potential ligands.

**PC(CB3)-25: Molecular Modeling – I** (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix -

Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

**PC(CB3)-26: Molecular Modeling – II** (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

**PC(CB3)-27: Drug Design Methods I - Ligand Based** (15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, $r^2$, $r^2$%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

**PC(CB3)-28: Drug Design Methods II - Structure Based.** (15hrs)

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

**Books suggested:**

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition

7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington, Pharmaceutical Press
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Wiley-Interscience, New York
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

**ELECTIVE –4B (ID PAPER)**

**PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry**

PC(CB4) -29: Water and Waste Water Treatment
PC(CB4) -30: Corrosion and its Control
PC(CB4) -31: Energy Sources
PC(CB4)- 32 Engineering Materials

**Learning Objectives:**

- Understand the causes and types of water hardness, differentiate between temporary and permanent hardness, and interpret hardness measurements.
- Identify common boiler issues, their causes, and effects, and evaluate methods for effective boiler water treatment.
- Explore various methods for treating saline water and wastewater, and assess their efficiency in practical applications.
- Highlight the global economic and environmental impacts of corrosion on industries and infrastructure.
- Explain corrosion theories, including chemical and electrochemical processes, and apply them to various metal environments.
- Describe corrosion reactions, focusing on oxidation, reduction, and the formation of corrosion products, to understand degradation mechanisms.
- Analyze coal's properties through proximate and ultimate analysis for combustion.
- Explore liquid fuels like petroleum and derivatives, studying refining processes and factors affecting quality.
- Understand cement composition, properties, setting processes, and preservation methods. Explore lime production and applications of plaster of Paris.
- Define criteria for lubricants, classify types, and discuss their properties such as viscosity and flash point.
- Classify refractories, analyze reasons for failures, explore glass manufacture, and introduce porcelain, enamels, and abrasives properties and applications.

**Course Outcomes:**

- Identify water hardness causes, quantify concentrations using appropriate methods, and differentiate between types.

- Analyze boiler issues like scaling and foaming, and propose effective water treatment solutions.
- Evaluate methods for treating saline water and wastewater, considering environmental impacts and efficiency in diverse applications.
- Evaluate corrosion risks, propose prevention strategies, and assess their implications.
- Apply chemical and electrochemical corrosion theories to predict and understand degradation mechanisms.
- Analyze factors influencing corrosion rates, develop mitigation strategies, and optimize corrosion control measures for diverse environments.
- Classify chemical fuels by physical state, assess their energy content, combustion properties, and environmental impacts.
- Analyze coal and petroleum through proximate and ultimate analysis, and explore refining processes and techniques.
- Evaluate properties, applications, and calorific values of liquid and gaseous fuels, including synthetic and alternative fuels.
- Understand Portland cement composition and chemical reactions for setting. Analyze decay mechanisms in cement concrete and propose preservation methods. Discuss lime production types and applications, including plaster of Paris.
- Evaluate lubricant types based on properties and applications. Interpret key lubricant characteristics such as viscosity and temperature properties.
- Analyze refractories classification and failure factors. Discuss glass manufacturing processes, raw materials, and applications.

**PC(CB4) -29:Water and waste water treatment** ( 15 hrs)

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electrodialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

**PC(CB4) -30: Corrosion and its control:** (15 hrs)

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal, electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods- design and material selection, cathodic protection, sacrificial anode, impressed current cathode. Surface coating methods: Surface preparation, metallic coatings, application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

**PC(CB4) -31: Energy sources:** (15 hrs)

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous). Solid fuels: coal, analysis of coal, proximate and ultimate analysis and their significance. Liquid fuels:

petroleum, refining of petroleum, cracking, reforming. Synthetic petrol - Bergius and Fischer-Tropsch's process, knocking, anti knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants.

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, $H_2$ as a non- polluting fuel.

**PC(CB4) -32: Engineering materials.** (15 hrs)

Cement: composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscocity.

Refractories: Classification, characteristics of good refractory, failure of refractories. Glass, glass making oxides and their functions, manufacture of glass. Porcelain, enamels, abrasives.

Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors ( Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

**Books suggested:**

1.Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2006).
2.Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2006).
3.Engineering Chemistry by B. Siva Shanker: Mc-Graw Hill publishing Company Limited, New Delhi (2006)
4.Engineering Chemistry by J.C. Kuriocose & J. Rajaram, Tata McGraw Hill Co. NewDelhi (2004)
5.Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company, (2008)
6.Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
7.Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
8.Applied Chemistry – A text book of engineering and Technology – Springar (2005)
9.Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2008)
10. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2008).

**ELECTIVE–4C (ID PAPER)**

**PAPER-IV CH(PC) 404T(CB5): Sugar Chemistry AND Sugar Technology**

PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar & Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

**Learning Objectives:**

- Understand the nomenclature, structures (Fischer, Haworth, conformational), and chemical reactivity of mono- and oligosaccharides, including reducing and non-reducing sugars.
- Learn about the chiral nature of sugars, stereochemical nomenclature, acyclic and cyclic structures, conformational analysis, and stereochemical transformations of sugars.
- Understand the structure, synthesis, and biosynthesis of sucrose, along with oligosaccharide synthesis and their optical properties.
- Learn about the uses of sugar chirons in organic synthesis, and the characteristics and applications of sugar byproducts like bagasse, molasses, and press mud.
- Understand various sampling techniques, moisture determination methods, and estimation techniques for total soluble solids and reducing sugars in sugar products.
- Learn about instrumental methods used in the sugar industry, including optical methods, potentiometry, pH meters, and polarimetry.
- Understand the principles of cane juice clarification, defecation, sulphitation, and the operations of various sugar processing equipment like juice heaters and centrifuges.
- Learn about the basic principles of management in the sugar industry, including production management, personnel administration, and organizational control.

**Course Outcomes:**

- Gain proficiency in identifying and analyzing the structures and reactivity of various sugars, including their stereochemistry and conformational properties.
- Develop skills in calculating conformational free energies, understanding optical rotations, and applying the general epimer rule and stereochemical transformation processes.
- Gain proficiency in determining the structures and synthesis pathways of sucrose and oligosaccharides, and interpreting 13C NMR spectroscopic data.
- Develop skills in utilizing sugar byproducts for various applications, including biogas production, fiberboard manufacturing, and fermentation processes.
- Gain proficiency in conducting sugar analysis using different methods, including Eynon & Lane, Luff & Schoorl, and Benedict's methods.
- Develop skills in using and understanding the working principles of instruments like potentiometers, pH meters, and polarimeters for sugar analysis.
- Gain proficiency in applying the principles of sugar technology, including cane juice processing and chemical control in milling and boiling house operations.
- Develop skills in management practices relevant to the sugar industry, including factory site location, plant layout, and production management.

**PC(CB5) -33: Advanced Sugar Chemistry:** (15 hrs)

Carbohydrate nomenclature. Fischer, Haworth and conformational structures of mono and oligo saccharides. Chemical reactivity of sugars. Reducing and non-reducing sugars. Chiral nature of sugars. R-S nomenclature, Fischer D-L nomenclature of sugars. Sugar enantiomers, diastereo isomers, epimers and enomers. Acyclic structure of sugars, determination of relative and absolute configuration of sugars. Cyclic forms of sugars. Conformational analysis of sugars. Hassel- Otter effect. Delta-two effect. Anomeric effect. Calculation of conformational free energies. Optical rotation, specific rotation and molecular rotation of sugars. General epimer rule. Relationship between rotation and conformation. Stereo chemical transformations. Mutarotation, enolization, isomerization, anhydride formation and reversion, pH stability of glucose and fructose, protection of sugar hydroxyls.

**PC(CB5) -34: Sugar & Sugar byproducts:** (15 hrs)

Structure determination of sucrose, synthesis of sucrose, biosynthesis of sucrose, chemical nature of sucrose. Oligo saccharide synthesis. Oligo saccharide optical rotating power (Hudson and Klyn rules). $^{13}C$ NMR spectroscopic data of glucose, fructose and sucrose. Uses of sugar chirons in organic synthesis. Sugar byproducts. Bagasse, molasses and press mud. Bagasse- characteristics and uses. Production of biogas, fiberboard and furfural. Press mud- extraction of cane wax, press mud and manure. Molasses- fermentation of molasses. Production of alcohol and rectified spirit.

**PC(CB5) -35:Methodology used in Sugar Analysis:** (15 hrs)

Sampling techniques. Determination of moisture in bagasse, molasses and cane sugar. Methods of estimation of total soluble solids in sugar and sugar house products. Optical methods of sugar analysis, sugar scales and normal weight. Estimation of reducing sugars and sugar present in cane juice by Eynon & Lane, Luff & Schoorl and Benedicts methods. Determination of sugars by Invertase method, Jackson- Gellis, Munsen- Walker's $Cu_2O$ and De Whalleys' volumetric method. Determination of Ash by Carbonate- Ash and Cuitometeric (Conductometric) methods. Determination of various other constituents present in raw sugars. Estimation and chemical composition of cane and its juice.

Instrumental methods of sugar industry- Static characteristics and Dynamic characteristics. Gas, liquid, vapor thermometers. Bimetallic thermometers and thermocouples. Electronic panometer, cuitometer. Introduction to pneumatic control systems and elements. Working principle and instrumentation methodology of potentiometer, pH meter, polarimeter and cuitometer.

**PC(CB5) -36: Sugar Technology and Basic Principles of Management:** (15 hrs)

Sugar Technology: Cane juice interaction, maceration and imbibition. Principles of cane juice clarification, defecation and sulphitation. Juice heaters, filters and reaprovation vaccum pans. Centrifuges. Sugar driers and molasses. Introductory treatment of chemical control (i) Milling Control and (ii) Boiling house control.

Management: Concept and philosophy of management in major and small-scale industries. Location of factory site and Lay out of plant. Joint stock companies. Co-operative Societies. Production management and control. Personnel administration, purchases and sales, organization and control.

**Books suggested:**

1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons
2. Determination of Food Carbohydrates, D. A. T. Southgate, Applied Science Publishers, London
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur

4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman
6. Text Book of Biochemistry, Lehninger
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot
9. Instrumental Methods in Sugar Industry, Eckman
10. Principles of Instrumental Analysis, Skoog and West
11. Technical Methods of Analysis, Griffith, McGraw Hill
12. Advanced Sugar Chemistry, R. S. Shellaxberges
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough
14. International Uniform Methods for Sugar Analysis, H. C. S. De Whelly

## IV SEMESTER PRACTICALS

**Note:** The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

**CH (PC) 451P: Paper-V (Chemical Kinetics)** 9hrs/week

**Course Objectives:**

- The learners should be able to validate the conceptual understanding acquired from the theory classes

**Learning Outcomes**: At the end of the course, the learners should be able to:

- **Explain** the principle behind the experiments performed in the laboratory
- **Plan** and **Perform** experiments and **Interpret** experimental results

♦ **Study of acetone-iodine reaction by spectrophotometry**

1. Order w.r.t.[ iodine]
2. Order w.r.t. [acetone]
3. Order w.r.t. [$H^+$]

♦ **Study of peroxydisulphate – iodide reaction by colorimetry**

♦ **Study of saponification of ethyl acetate by conductometry:**

1. Overall order of the reaction
2. Order w.r.t. [ethyl acetate]
3. Order w.r.t. [NaOH]

♦ **Study of solvolysis of t-butylchloride by conductometry**:
effect of solvent dielectric constant/
polarizability (methanol/water mixture) on the rate of solvolysis

♦ **Study of oxidation of primary alcohols by dichromate by spectrophotometry**:
Application of Taft equation

**CH (PC) 452P: Paper-VI (Instrumentation)** 9 hrs/week

**Course Objectives:**

- ❖ The learners should be able to validate the conceptual understanding acquired from the theory classes

**Learning Outcomes**: At the end of the course, the learners should be able to:

- ➢ **Explain** the principle behind the experiments performed in the laboratory
- ➢ **Plan** and **Perform** experiments and **Interpret** experimental results
- ➢ **Record data and analyze** it obtained from Instrumental operation and experimentation.

**Spectrophotometry:**

- ♦ Estimation of Cu(II) using EDTA
- ♦ Estimation of Fe(III) using thiocyanate
- ♦ Estimation of Fe(II) using 1,10-phenanthroline
- ♦ Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- ♦ Simultaneous determination of dichromate and permanganate in a mixture
- ♦ Spectrophotmetric titrations: Cu(II) vs EDTA
  Fe(II) vs 1,10-phenanthroline
- ♦ Composition of Cu(II) – EDTA complex by Job's method
- ♦ Composition of Fe(II) – phenanthroline complex –Job's method, mole ratio, slope ratio method.
- ♦ Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex
- ♦ Determination of $pK_a$ of methyl red indicator
- ♦ Estimation of Mn(II) by spetrophotometry using periodate.

**Potentiometry:**

- ♦ Potentiometric titrations:

1. Weak acids vs strong base and calculation of dissociation constants
2. Mixture of strong and weak acids vs strong base
3. Dibasic acid vs strong base
4. Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
   - ♦ Fe(II) vs $MnO_4^-$
   - ♦ Fe(III) vs EDTA
   - ♦ Mixture of halides vs $AgNO_3$
   - ♦ Mixture of KI and KSCN vs $AgNO_3$

**Polarography:**

- ♦ Estimation of $Pb^{2+}$, $Cd^{2+}$ and $Ni^{2+}$ separately and in a mixture.

**Suggested books:**

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B. Yadav