Ordinance No. :- V-141-B-16

(Approved in Academic Council meeting held on 11.03.2026 Proposed to be ratified in forthcoming executive council)

Evaluation Scheme and Syllabus

of

M.Sc. INDUSTRIAL CHEMISTRY

TWO – YEAR POST GRADUATE

PROGRAM

(AS PER NEP-2020)

Keral Verma Subharti College of Science

Swami Vivekanand

SUBHARTI UNIVERSITY

Meerut

Effective from 2025-2026

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

Programme Educational Objectives (PEO)

PEO 1: To deliver advanced concepts in Chemistry covering topics in Analytical, Inorganic, Organic and Physical Chemistry, while also reinforcing the fundamental concepts.

PEO2: To make students proficient in advanced laboratory techniques, enabling them to independently plan and conduct experiments as well as to work as a team.

PEO 3: To expose the students to a range of analytical methods using modern instrumentation, enabling them to analyze results at a higher level.

PEO 4: To make them as competent industrial chemists with strong theoretical knowledge and practical skills in chemical sciences, enabling them to work effectively in chemical, pharmaceutical, polymer, petrochemical, materials, and related industries.

PEO5: To develop ethical behavior, environmental responsibility, and adherence to industrial safety, quality, and regulatory standards in professional practice.

Programme Outcomes (PO's)

PO1: Attain sound knowledge about the fundamentals and applications of chemical and scientific theories.

PO2: Gain knowledge and understanding of reaction mechanisms, complex chemical structures, instrumental method of chemical analysis, molecular rearrangements and separation techniques.

PO3: Acquire general, technical, and professional skills to accomplish tasks in research, industry or academia.

PO4: Apply of knowledge and skills in addressing social economic and environmental problems.

PO5: Demonstrate in-depth understanding of chemical sciences, industrial processes, reaction mechanisms, and material properties relevant to chemical and allied industries

PO6: Apply chemical principles to design, scale up, monitor, and optimize industrial processes in areas such as polymers, pharmaceuticals, petrochemicals, dyes, and environmental chemistry.

PSO1 : Apply modern research techniques to investigate complex chemical phenomena and solve practical problems.

PSO2 : Implement safe laboratory and industrial procedures, follow environmental and sustainability guidelines, and understand relevant quality and regulatory standards

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

SWAMI VIVEKANAND SUBHARTI UNIVERSITY, MEERUT							
KERAL VERMA SUBHARTI COLLEGE OF SCIENCE							
M.Sc. Industrial Chemistry Program offered by Department of Chemistry (Session 2025-26 onwards)							
		I	**II**	**Internship after II Semester**	**III**	**IV**	**Total**
1	Core Course	16	16	**4**	8	4	44
2	Elective (DEC)	-	-		8	8	16
3	PC/Dissertation/Project Work	8	8		8	12	36
4	SEMINAR/VAC/OEC/EEC/CHM	2 (SEMINAR)	2 (CHM)		2 (OEC)	2 (EEC)	8
	Total	26	26		26	26	108

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

List of all Courses under different categories for M.Sc. Industrial Chemistry

Semester	Course Type	Course Code	Course Name	Credits
Semester I	Core Course - 1	MSIC -101	Physical Chemistry - I	4
	Core Course - 2	MSIC -102	Inorganic Chemistry - I	4
	Core Course - 3	MSIC -103	Organic Chemistry - I	4
	Core Course - 4	MSIC -104	Analytical Chemistry - I	4
	Practical Course -1	MSIC -105P	Qualitative & Quantitative Analysis of Inorganic Compounds	4
	Practical Course - 2	MSIC -106P	Physical Chemistry Laboratory	4
	SEMINAR	MSIC -107		4
Semester II	Core Course - 5	MSIC -201	Physical Chemistry - II	4
	Core Course - 6	MSIC -202	Inorganic Chemistry - II	4
	Core Course -7	MSIC -203	Organic Chemistry – II	4
	Core Course - 8	MSIC-204	Analytical Chemistry - II	4
	Practical Course -3	MSIC -205P	Qualitative & Quantitative Analysis of Organic Compounds	4
	Practical Course - 4	MSIC -206P	Analytical Method Development and Validation	4
	CHM	CHM	Intellectual Property Rights	2
Semester III	Core Course - 9	MSIC -301	Chemistry of Agrochemicals, Textiles and Polymers	4
	Core Course - 10	MSIC -302	Chemistry of Industrial Minerals	4
	DISCIPLINE ELECTIVE COURSE -1	MSIC -303A/ MSIC -303B/ MSIC -303C/ MSIC -303D	Bioinorganic Chemistry / Bioorganic Chemistry/Biophysical Chemistry/Natural Products Chemistry	4
	DISCIPLINE ELECTIVE COURSE -2	MSIC -304A/ MSIC -304B/ MSIC -304C/ MSIC -304D	Nanochemistry / Organometallic Chemistry / Quantum Chemistry/ Surface Chemistry	4
	Practical Course -5	MSIC -305P	Industrial Chemistry	4

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

			Laboratory -1	
	Practical Course -6	MSIC -306P	Industrial Chemistry Laboratory -2	4
	OEC		To Be selected from the Bucket of Courses	2
Semester IV	Core Course - 11	MSIC - 401	Pharmaceutical Chemistry	4
	DISCIPLINE ELECTIVE COURSE - 3	MSIC -402A/ MSIC -402B/ MSIC -402C/ MSIC -402D	Green Chemistry/ Polymer Chemistry/ Material Chemistry/Computational Chemistry	4
	DISCIPLINE ELECTIVE COURSE - 4	MSIC -403A/ MSIC -403B/ MSIC -403C/ MSIC -403D	Medicinal Chemistry/ Environmental Chemistry/ Photochemistry/ Supramolecular Chemistry	4
	DISSERTATION	MSIC -404	Project	12
	EEC			2

Program Name -M.Sc. Industrial Chemistry													
Batch:2025-27							**SEMESTER:I**						
S.No.	**Course Type**	**Course Code**	**Course Name**	**Teaching Load**			**Credits**	**Internal Assessment**				**External Assessment**	**Total**
				L	**T**	**P**							
THEORY and PRACTICAL SUBJECTS								**CLASS PARTICIPATION**	**Quiz/PPT /Assignment (10)**	**Mid Sem Test (15)**	**TOTAL**	**End Sem Exam (70)**	
1	CORE COURSE-1	MSIC-101	Physical Chemistry-I	4	0	0	4	5	10	15	30	70	100
2	CORE COURSE-2	MSIC-102	Inorganic Chemistry-I	4	0	0	4	5	10	15	30	70	100
3	CORE COURSE-3	MSIC-103	Organic Chemistry-I	4	0	0	4	5	10	15	30	70	100
4	CORE COURSE-4	MSIC-104	Analytical Chemistry - I	4	0	0	4	5	10	15	30	70	100
5	PRACTICAL COURSE-1	MSIC-105P	Qualitative & Quantitative Analysis of Inorganic Compounds	0	0	8	4	5	10	15	30	70	100
6	PRACTICAL COURSE-2	MSIC-106P	Physical Chemistry Laboratory	0	0	8	4	5	10	15	30	70	100
7	SEMINAR	SEMINAR		0	0	4	2	4	4	7	15	35	50
TOTAL CREDITS / ASSESSMENT							**26**	34	64	97	195	455	**650**

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

Program Name -M.Sc. Industrial Chemistry														
Batch:2025-27							**SEMESTER:II**							
S.No.	**Course Type**	**Course Code**	**Course Name**	**Teaching Load L**	**T**	**P**	**Credits**	**Internal Assessment**				**External Assessment**	**Total**	**Remark**
THEORY and PRACTICAL SUBJECTS								**CLASS PARTICIPATION**	**Quiz/PPT/Assignment (10)**	**Mid Sem Test (15)**	**TOTAL**	**End Sem Exam (70)**		
1	CORE COURSE -5	MSIC-201	Physical Chemistry-II	4	0	0	4	5	10	15	30	70	100	
2	CORE COURSE -6	MSIC-202	Inorganic Chemistry-II	4	0	0	4	5	10	15	30	70	100	
3	CORE COURSE -7	MSIC-203	Organic Chemistry-II	4	0	0	4	5	10	15	30	70	100	
4	CORE COURSE -8	MSIC-204	Analytical Chemistry - II	4	0	0	4	5	10	15	30	70	100	
5	PRACTICAL COURSE -3	MSIC-205P	Qualitative & Quantitative Analysis of Organic Compounds	0	0	8	4	5	10	15	30	70	100	
6	PRACTICAL COURSE -4	MSIC-206P	Analytical Method Development and Validation	0	0	8	4	5	10	15	30	70	100	
7	CHM	CHM	Intellectual Property Rights	2	0	0	2	4	4	7	15	35	50	
TOTAL CREDITS / ASSESSMENT							**26**	34	64	97	195	455	**650**	

1. AN INTERNSHIP COURSE OF 4 CREDITS OF 4-6 WEEKS DURATION DURING SUMMER VACATION, AFTER IIND SEMSTER TO ENHANCING THE EMPLOYABILITY OR AN DEVELOPING THE RESEARCH APTITUDE.

2. THE POST GRADUATE DIPLOMA IN CHEMISTRY WILL BE AWARDED HERE AFTER THE SUBMISSION OF INTERNSHIP COURS

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Semester I

Course Name: Physical Chemistry - I	Course Code: MSIC-101
Credit 4	Core Course -1

Course Objectives

1. To provide the understanding of physical states of matter and their practical applications. To define how the initially primitive models of real gases in physical chemistry are elaborated to take into account more detailed observations.
2. To understand the concept of partial molar quantities and their variation with temperature and pressure.
3. The concept of ensembles, partition function and their applications in studying gaseous molecules.
4. To understand the concept and different theories of ions and electrolyte interactions
5. To discuss the theoretical aspects of chemical kinetics and the importance of rate equations and different theories for studying the kinetics of complex reactions.
6. To provide an in-depth analysis of various phenomenon, laws and applications of States of Matter, Thermodynamics, Electrochemistry, Phase Equilibrium and Chemical Kinetics.

Course Outcomes

CO1: Understand the detailed concept of liquid and gaseous state and the structural features of solid state material by having complete knowledge of X-ray diffraction and its analysis.
CO2: Understand the application of second law of thermodynamics and the concept of third law of thermodynamics.
CO3: Familiarize with the applications of partition function and statistics in understanding the thermodynamics of molecules.
CO4: Understand the concept of electrical double layer at the electrode electrolyte interface by studying different proposed models of it.
CO5: Understand the detailed concepts of kinetics and its applications, Influence of physical and chemical parameters on reaction rates in solutions
CO6: Do the in-depth analysis of various phenomenon and laws of States of Matter, applications of Thermodynamics, Electrochemistry and Chemical Kinetics and different functions of statistical thermodynamics.

Course Description

The course is framed to give broad view of states of matter, chemical potential, concepts of electrical double layer in solutions and various models to explain it. Concept of existence of different phases in the form of phase diagrams and their existence with changing variables.

Outline Syllabus

Unit 1 States of Matter

(a) Gaseous State : Maxwell–Boltzmann distribution of molecular velocities of gases.
(b) Liquid State: Structure of liquids, Radial distribution functions, Monte–Carlo method, Molecular dynamics.
(c) Solid State: Types of solids, Debye- Scherrer method of X-ray structure analysis of crystals, indexing of reflections, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electron density, Rietveld analysis, particle size of crystallites.

Unit 2 Thermodynamics

Essentials of thermodynamics, fugacity, standard state of real gases, the relation between fugacity and pressure, Partial molar quantities, chemical potential and Gibbs Duhem equation.

Classius – Clayperon equation; law of mass action and its thermodynamic derivation, variation of chemical potential with temperature and pressure, chemical potential for an ideal gas, deterrmination of partial molar volume, thermodynamic functions of mixing (free energy, entropy, volume and enthalpy), third law of thermodynamics, residual entropy, meaning and scope of irreversible thermodynamics.

Unit 3 Statistical Thermodynamics

Concept of distribution, Thermodynamic probability and most probable distribution. Ensembles, Canonical, grand canonical and microcanonical ensembles.

Partition function - Translational, Rotational, Vibrational and Electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions.

Heat capacity behaviour of solids - Chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law, Bose-Einstein statistics - distribution law, Evaluation of Lagrange's undeterrmined multipliers.

Unit 4 Electrochemistry

Debye-Huckel theory of ion- ion interactions, Debye Huckel limiting law of activity coefficients and its limitations.

Debye - Huckel - Onsager treatment for aqueous solutions and its limitations, Wein effect, Debye – Falkenhagen effect.

The electrode-electrolyte interface: The electrical double layer -The Helmholtz-Perrin parallel plate model, the Gouy-Chapman diffuse-charge model and the Stern model, excess function.

Unit 5 Chemical Kinetics

Simple collision theory of reaction rates, Arrhenius equation and activated complex theory (ACT), thermodynamic treatment, chain reactions (hydrogen halogen reactions) decomposition of N_2O_5.

Theory of unimolecular reactions: Lindemann – Hinshelwood mechanism of unimolecular reactions, RRKM and Slater treatment.

Factors affecting rate of chemical reactions in solution Effect of solvent and ionic strength (Primary salt effect) on rate constants, secondary salt effect.

Reference Books

1. Atkins P. W., Physical Chemistry, Oxford University Press, New York.
2. Kapoor K. L., Textbook of Physical Chemistry (Volume 1)
3. Kapoor K. L., Textbook of Physical Chemistry (Volume 3)
4. Kapoor K. L., Textbook of Physical Chemistry (Volume 5)
5. Puri, Sharma and Pathania, A Textbook of Physical Chemistry, Vishal Publishing Cor

Semester I

Course Name: Inorganic Chemistry - I	Course Code: MSIC-102
Credit 4	Core Course -2

Course Objectives

1. To provide an insight into bonding and structure of coordination compounds.
2. To explain the spectral and magnetic behaviour of coordination compounds.
3. To provide a thorough knowledge about the chemistry and application of inner transition metals.
4. To discuss about various spectroscopic methods for structure elucidation of inorganic compounds.
5. To explain the basics of radioactivity as well as various radio analytical techniques.
6. To impart knowledge about structure, bonding and application of inorganic compounds and radio chemistry.

Course Outcomes

CO1: Explain the various theories of metal –ligand bonding.
CO2: Explain the electronic spectra and magnetic properties of transition metal complexes.
CO3: Interpret the EPR and Mossbauer spectra.
CO4: Illustrate the chemistry and uses of inner transition metals.
CO5: Know about various radio-analytical techniques.
CO6: Gain knowledge about of various aspects of modern inorganic chemistry.

Course Description

This course includes basic concepts of metal –ligand bonding, magnetic and electronic properties of coordination compounds and their characterization techniques. Chemistry of inner transition metals and nuclear chemistry are also discussed in this course.

Outline Syllabus

Unit 1 Metal-ligand Bonding

Overview of crystal field and ligand field theories of 4-, 5-and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal-bipyramidal and cubic complexes. Measurement of CFSE (d1 to d10) in weak and strong ligand fields, JahnTeller distortion, nephelauxetic series

Molecular orbital theory (MOT) of coordination compounds: Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both s and p bonding, angular overlap model.

Unit 2 Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Interpretation of electronic spectra, Orgel diagrams, Tanabe-Sugano diagrams for transition metal complexes (d1 - d 9 states), calculations of Dq, B and β parameters.
Charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information.

Anomalous magnetic moments, magnetic exchange coupling, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon. Effect of temperature on their magnetic properties.

Unit 3 Chemistry of Inner Transition Elements

General discussion on the properties of the f-block elements.

Redox, Spectral and Magnetic properties.

Use of Lanthanide compounds as shift reagents. Photophysical properties of Lanthanide complexes.

Unit 4 Characterization Techniques

EPR spectroscopy-basic principle, hyperfine and superhyperfine lines, anisotropy, g values, application in selected inorganic compounds.

Mossbauer Spectroscopy-Gamma ray emission and absorption by nuclei, Mossbauer effect -conditions, Doppler effect, instrumentation, chemical shift examples, quadrupole effect.

Use of Mössbauer spectra in chemical analysis, typical spectra of iron and tin compounds. Optical rotatory dispersion (ORD) and circular dichroism (CD).

Unit 5 Nuclear Chemistry

Nuclear structures and nuclear stability. Nuclear models; radioactivity and nuclear reactions. Detection and measurement of radiation. Tracer techniques.

Study of chemical reactions, isotope exchange reactions, kinetic isotope effect, nuclear activation analyses, Principle of nuclear detection, gas detector, ionization chamber, proportional and G. M. detector.

Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters.

Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

Reference Books

1. Inorganic Chemistry, J.E. Huhey, Harper & Row
2. Concise Inorganic Chemistry,J. D. Lee, Elbs with Chapman and Hall, London.
3. The Chemical bond, J.N.Murre l, SFA Kettle and JM. Tedder, Wiley, New York.
4. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Semester I

Course Name: Organic Chemistry - I	**Course Code: MSIC-103**
Credit 4	**Core Course -3**

Course Objectives

This course aims to
1. Analyze delocalized chemical bonding mechanisms, including resonance, hyperconjugation, aromaticity, and tautomerism.
2. Examine thermodynamic and kinetic requirements influencing reaction mechanisms and apply key concepts such as the Hammond postulate, Curtin-Hammett principle, and catalytic processes in organic reactions.
3. Differentiate between classical and non-classical carbocations and their rearrangements and explain the reactivity of carbanions, free radicals, carbenes, nitrenes, and benzynes.
4. Identify elements of symmetry and chirality in organic molecules and understand stereochemical concepts such as stereospecificity, stereoselectivity, and asymmetric synthesis.
5. Perform conformational analysis of cyclic systems and determine their effects on chemical reactivity. Also, evaluate stereochemical factors.

Course Outcomes

Upon successful completion of this course, students will be able to
CO1: Explain and apply delocalized bonding concepts (resonance, hyperconjugation, and tautomerism) in organic molecules and determine aromaticity in organic compounds using Huckel's rule and modern aromaticity principles.
CO2: Predict the reaction mechanism of organic transformations based on kinetic and thermodynamic considerations.
CO3: Identify and analyze key reaction intermediates (carbocations, carbanions, free radicals, carbenes, and benzynes) and their reactivity.
CO4: Apply stereochemical principles to understand molecular chirality, stereoselectivity, and asymmetric synthesis strategies.
CO5: Perform conformational analysis of cyclic systems and predict their impact on reaction outcomes, and evaluate the role of neighboring group participation in substitution and elimination reactions.
CO6: Gaining expertise in bonding, reaction mechanisms, intermediates, and stereochemistry, enabling them to analyze structures, predict reactivity, and apply concepts in research and industry.

Course Description

This course provides an in-depth exploration of advanced organic chemistry, focusing on bonding, reaction mechanisms, intermediates, and stereochemistry. It covers delocalized chemical bonding, aromaticity, and reaction pathways, emphasizing kinetic and thermodynamic principles. The study of key reaction intermediates such as carbocations, carbanions, and free radicals enhances the understanding of organic transformations. Stereochemical concepts, including chirality, conformational analysis, and asymmetric synthesis, are explored to predict molecular behavior in various reactions. Through theoretical and applied perspectives, this course equips students with the skills necessary for research and industrial applications in organic chemistry

Outline syllabus

Unit 1 Nature of Bonding in Organic Molecules

Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, tautomerism;

Criteria for aromaticity: Huckel's 4n+2 electron rule for benzenoid and nonbenzenoid aromatic compounds; Application in carbocyclic and heterocyclic systems, annulenes, heteroannulene, fullerenes, C-60, cryptates, azulenes.

Current concepts of aromaticity: Anti-aromatic, nonaromatic and homoaromatic compounds, Effect of tautomerism and hyperconjugation on aromaticity.

Unit 2 Reaction Mechanism - Structure and Reactivity

Types of reaction mechanisms: substitutions, eliminations, additions, rearrangements, thermodynamic and kinetic requirements.

Hammond postulate, Curtin-Hammett principle, transition states and intermediates, catalysis: electrophilic catalysis, acid and base catalysis.

Methods of determination of reaction mechanism methods: Detection of intermediates, Stereochemical and chemical evidences, Identification of products, isotopic labelling and cross-over experiments.

Unit 3 Reaction Intermediates

Carbocations: Classical and nonclassical, phenonium ions, norbornyl system, common carbocation rearrangement: Wagner Meerwein rearrangement, Demjonove rearrangement, and Pinacol-pinacolone rearrangement.

Carbanions: formation, stability and their reactions. HSAB principle and its applications.

Free radicals: formation, stability and reactions, cage effects, radical cations and radical anions;

Carbene: Synthesis, structure and reactions of singlet and triplet carbene, nitrenes, Benzyne.

Unit 4 Stereochemistry I

Elements of symmetry, chirality (centre, axis, and plane), molecules with more than one chiral center, threo and erythro isomers, optical purity.

Topicity of ligands and faces and their nomenclature, stereogenecity, chirogenicity and pseudo symmetry, stereospecific and stereoselective reactions.

Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction- substrate, reagent and catalystcontrolled reactions; deterrmination of enantiomeric and diastereomeric excess; enantio-discrimination, Resolution – optical and kinetic.

Unit 5 Stereochemistry II

Conformational analysis of cyclic systems: Cyclohexane and its derivatives (mono- and di-substituted), fused (decalins) and bridged bicyclic systems.

Nucleophilic addition to carbonyl group: Cram, Franklin Ahn Model, Cieplak effect, Effect of conformation on the reduction of cyclic ketones, nucleophilic substitution on cyclohexane substrates, cyclohexane epoxide formation and opening.

Elimination reactions of cyclohexyl halides, de-amination of 2-aminocyclohexanols, elimination vs substitution competition and neighboring group participation reactions of acyclic and cyclic molecules.

Reference Books

1.Organic Chemistry, R. T. Morrison and R. N. Boyd, (1992) 6th Edition, Prentice-Hall.
2. Reaction Mechanism in Organic Chemistry, (1976) 1 st Edition, S. M. Mukherji and S. P. Singh, Macmillan.
3. Stereochemistry, P. S. Kalsi, (1994), 2nd Edition, New Age International.

Semester I

Course Name: Analytical Chemistry - I	Course Code: MSIC-104
Credit 4	Core Course - 4

Course Objectives

1. Provide and enrich the students to analytical techniques, various types of errors knowingly/ unknowingly introduced, accuracy and confidence limit in analytical process.

2. Provide detailed insight of chemical equilibrium and its effect in chemical analysis of analyte.

3. Provide detailed technical knowledge of various chromatogaraphic separation techniques based on physical state, contact and separation mechanism.

4. Provide detailed technical knowledge of gas, thin layer chromatographic, integrated LC-MS and GC-MS separation techniques for qualitative and quantitative analysis.

5. Enable the students to study the thermal behaviour of different compounds and study temperature dependent decomposition process and structural elucidation of unknown analyte.

6.Estimate the temperature dependent weight loss in compound and model and optimize suitable temperature condition for further chemical processing.

Course Outcomes

CO1: Apply the knowledge of analytical techniques to minimize the error and report the outcomes of analysis with high precision and accuracy.

CO2: Understand the role of different analytical techniques used for the separation of compounds present in very small quantity.

CO3: Understand the role of chemical equilibrium in chemical analysis.

CO4: Segregate and select the suitable indicator for measurement of pH,.

CO5: Purify the various compounds for their further detailed structural elucidation and molecular mass analysis.

CO6: To learn analytical tools involving Chromatographic methods and thermo-analytical instruments of a lab for the identification of equilibrium process.

Course Description

Analytical chemistry I emphasizes on various factors as - types of errors, accuracy and precision in chemical analysis, concepts of chemical equilibrium and its effects on qualitative and quantitative estimation, Chromatographic separation and Thermal analysis.

Outline syllabus

Unit 1 Introduction to Analytical Chemistry

Scope & objectives of Analytical chemistry and chemical analysis, Classification of analytical methods. Errors in chemical analyses- Accuracy and precision.

Types of error-determinant, indeterminate and gross. Nature of random errors, statistical treatment of random errors, standard deviation of calculated results, reporting of calculated data.

Unit 2 Concept of Equilibrium

General treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases.

Activity and activity coefficient; Effect of electrolytes on chemical equilibria, Calculation of pH.
Constructing titration curves from charge balance and mass balance equations, Acid-base titrations and theory of pH indicators.

Unit 3 Chromatographic Methods – I

General principle, classification of chromatographic methods based on physical state, contact and separation mechanism.

Nature of partition forces. Chromatographic behavior of solutes. Chromatographic resolution, selectivity factor and column efficiency.

Column chromatography: Nature of column materials, Preparation of the column, Solvent systems, detection methods and applications.

Unit 4 Chromatographic Methods - II

Gas chromatography- principle, experimental technique, carrier gas, sample injection, column, detector and application.

High Performance Liquid Chromatography (HPLC): instrumentation- solvent and reservoirs, pumping system, sample injection, Column, detectors

Thin layer chromatography: coating of materials, preparation of TLC, Solvents, methods of detection and applications. Theory and application of LC-MS, Pyrolysis GC-MS, Thermal Desorption GC-MS.

Unit 5 Thermal Analysis

Principle, different methods of thermal analysis,

i) Thermo gravimetric methods of analysis (TG/DTG):
Instrumentation, thermogram and information from thermogram, factors affecting thermogram, applications TGA for quantitative analysis (TG analysis of $CaC_2O_4.H_2O$, $CuSO_4.5H_2O$, dolomite ore, etc.)
Problems based TGA,

ii) Differential Thermal Analysis (DTA):
Instrumentation, general principles, differential thermogram, DTA and TG curve together, Applications (DTA analysis of mixture of polymers, DTA of CaC_2O_4 H_2O, DTA of $CuSO_4$. $5H_2O$).

iii) Differential Scanning Calorimetry (DSC):
Principle, Instrumentation, and Applications (DSC curve of polyethylene terephthalate, DSC curve for isothermal crystallization of polyethylene, DSC of phenacetin), thermometric titrations, Evolved gas analysis.

Reference Books

1.Analytical Chemistry-An Introduction, 7th Edition,D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Saunders College Publishing, Philadelphia, London.
2. Modern Methods of Chemical Analysis, 2nd Edition,R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, John Wiley, New York.
3. Analytical Chemistry, 5th Edition,G. D. Christian, John Wiley & Sons, New York.
4. Analytical Chemistry: Principles, 2nd Edition,J. H. Kennedy, Saunders Holt, London.

Semester I

Course Name: Qualitative & Quantitative Analysis of Inorganic Compounds	Course Code: MSIC-105P
Credit 4	Practical course -1

Course Objectives

1. To find the individual strengths of acids and salts via thermometric titrations, conductometric titrations, precipitation titrations and pH metric titrations.
2. Find the heat of neutralization using Calorimetry.
3. To calculate the dissociation tendency of the acids.
4. To construct the phase diagrams of binary and ternary systems.
5. To learn software handling for chemistry problems.

Course Outcomes

Students will be able to –
CO1: To imply various types of titrations for quantitative analysis.
CO2: Construct the phase change behaviour in graphical form.
CO3: To carry out conductometric and potentiometric titrations.
CO4: To find the acidity strength accurately.
CO5: Utilize computational tools for solving chemical problems.
CO6: To imply titrations, Calorimetry, computational and phase change phenomena towards appropriate quantitative and qualitative assessment of the physical process.

Outline syllabus

Quantitative Analysis – I

- To determine the concentration of two acids, HCl and ethanoic acid, by thermometric titration and use it to calculate the enthalpy change of neutralization.
- To study precipitation titration between KCl and $AgNO_3$ conductometrically and deterrmine the strength of the given solution of $AgNO_3$.

Qualitative Analysis – II

- 1.Qualitative test for carbohydrates.
- 2. Qualitative test for lipids.
- 3. Qualitative test for amino acid and proteins.

Quantitative/Qualitative Assessment – I

- To determine the strength of strong acid and weak acid conductometrically by titrating against standard NaOH solution.
- To deterrmine the strength of H_3PO_4 by titration with standard NaOH using pH meter.

Quantitative/Qualitative Assessment –II

- To study the separation of dyes by thin layer chromatography (TLC).
- To determine the amount of $BaCl_2$ in a given solution by conductometric titrations.
- Study the conductometric titration of hydrochloric acid with sodium carbonate.

Preparation and characterization of the following inorganic compounds:

(i) Tetramminecupricsulphate [Cu(NH3)4]SO4 .H2O
(ii) Sodium cobaltinitrite , Na3[Co(NO2)6]
(iii) Potassium chromioxalate , K3[Cr(C2O4)3].

Reference Books

1. O.P. Pandey, D.N. Bajpai, S.Giri, " Practical Chemistry", S. Chand & Co.
2. Vogel's "Textbook of quantitative Analysis", Pearson
3.Practical Organic Chemistry: Preparations and Quantitative Analysis" by Mann and Saunders
4. Natural Products: A Laboratory Guide" by Raphael Ikan

Semester I

Course Name: Physical Chemistry Laboratory	Course Code: MSIC-106P
Credit 4	Practical course -2

Course Objectives

Understand and apply solvent extraction techniques for the quantitative analysis of bioactive compounds such as caffeine, carotenoids, and beta-carotene from natural sources.

Gain proficiency in spectroscopic methods like UV-Visible spectroscopy and FTIR for purity analysis and quantification of extracted compounds.

Acquire knowledge of flame photometry for the determination of alkali metals (Na^+, K^+) in environmental samples and perform regression and calibration curve analyses.

Master quantitative Thin Layer Chromatography (TLC) and paper chromatography methods, including color separation, elution, and quantification by colorimetry.

Understand High-Performance Liquid Chromatography (HPLC) operation, including mobile phase and column selection, chromatogram interpretation, and quantitative and qualitative analysis using peak area and height.

Understand Thermogravimetric Analysis (TGA) for studying thermal decomposition of substances and quantitative determination of components in ores and hydrates.

Course Outcomes

At the end of course students should be able to
CO1: Define various terms involved in practical methods of analysis.
CO2: Explain the instrumentations of colorimeter, spectrophotometer, photoflurometer, TGA, HPLC, Flame-photometer, CV, etc.
CO3: Apply/select method / instrumental parameters for analysis of the given sample.
CO4: Explain / describe basic principles of chromatography and different instrumental methods of analysis. Able to handle instruments according to SOP.
CO5: Differentiate among the various analytical methods / techniques of chemical analysis and verify theoretical principle practically or apply theory to explain practical observations.
CO6: Maintain a proper record of analytical data in notebook.
Observer personal safety in laboratory and able handle all chemicals, instruments, etc safely in laboratory.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Outline syllabus

Any 12 Experiments from the given list

1. Absorption spectra of organic compound.

2. To find out the surface tension of the given liquid by drop weight method at room temperature.

3 To determine the λmax of a given sample by visible spectrophotometer.
4. Determination of the concentration of unknown sample with the help of U.V visible spectrophotometer.

5. Solid Phase Extraction: Isolation of amino acids from aqueous sample using ion exchange resin and their identification by colorimetric test (very dilute glycine solution can be used as an example of alfa amino acid)

6. Pre-concentration using solid phase extraction on ion exchange cartridge and estimation. You can choose any metal ion which is present below detection limit. You will do preconcentration using ion exchange resin and will estimate by AAS or aqueous colorimetry (not solvent extraction). Example: Preconcentration of Cu(II) from brine (one can use aqueous solution of Cu(II) solution with less than 0.5 ppm conc.) and its estimation using R-Nitroso salt .

7. Flame photometric analysis of water /soil sample for Na+ and K+ by calibration curve method (give regression analysis for both curves) .

8 . Determination of available chlorine from bleaching powder.

9. Determination of Ni2+ using DMG by Gravimetric method.

10. Selective estimation of SO4 2- in presence of chloride from water sample or any other sample by calibration curve and its confirmation by turbidimetric titration method (give regression analysis for both curves).

11. Estimation of quinine sulphate from tablet by calibration curve and its confirmation by standard addition method.

12. Separation of Colours by TLC / Paper chromatography, their isolation by elution from paper or TLC and quantification by colorimetry.

13. Analysis of the Composition of a Mixture of Nitroanilines by Thin-Layer Chromatography and Ultraviolet/Visible Spectrometry.

14. Demonstration Practical by Mentori. Handling of HPLC equipment, choice of mobile phase and column,

sample preparation. ii. Record the chromatogram of pure substance and study

a) Effect of conc. on peak area and peak height

b) from retention time and length of column calculate number theoretical plates from.

c) Qualitative analysis – spiking method and by using retention time

d) Quantitative analysis by comparing peak height of sample with standard as well as by comparing peak area of sample with standard.

15. Demonstration Practical by Mentor Study of GC chromatogram: Record the TGA of pure $NaHCO_3$ (room temp to 300 °C). Explain different characteristics of thermogram and quantitative analysis by TGA. Explain how thermal decomposition reaction can be predicted from wt. loss.

16. TGA analysis of dolomite ore for $CaCO_3$ and $MgCO_3$ content.

17. Cyclic voltammetric study of Fe(II)/Fe(III) system. Basic principle and calculation of basic parameters from CV.

18. Construct graphite electrode using graphite rod from the dry pen-cell. Perform redox titration between Fe(II) and $KMnO_4$ using graphite electrode and calomel as reference electrode. Perform same titration using Pt electrode and calomel electrode. Report does Pt can be replaced by graphite or not. Give the reasons.

Reference Books

1. Vogel's Textbook of Quantitative Chemical Analysis, 6 th Ed

2. Indian Pharmacopeia, 2007

3. Chemical Separations Principle techniques and Experiments, Clifton E Meloan, Wiley Interscience.

4. Separation, Preconcentration and Spectrophotometry in Inorganic Analysis, by Z. Marczenko and M. Balcerzak, Analytical Spectroscopy Library – 10, Elsevier

5. Standard methods for the examination of water and wastewater, 23rd Ed. Roger B. Baird, Andrew D Eaton, Eugene W. Rice, American Public Health Association, Americal water works association, Water environment federation.

6. Biochemical Methods, Third Edition, By S Sadashivan, A. Manickam; New Age International Publishers

7. Extraction technique in Analytical Science, John R. Dean, Wiley 8. Experiments in modern analytical chemistry, D. Kealey, Springer Science Business media, 1986.

8.https://chem.libretexts.org/Courses/University_of_California_Davis/UCD_Chem_9_Lab_Manual/Lab_1%3A_Cyclic_Voltammetry

10.Cyclic Voltammetry Experiment James J. Van Benschoten. Jane Y. Lewis, and William R. Heineman, Journal of Chemical Education, Volume 60, Number 9, September 1983 (772-776) and Volume 60 Number 9 September 1983 (702-706)

11. Analysis of Soft Drinks: UV Spectrophotometry, Liquid Chromatography, and Capillary Electrophoresis, Journal of Chemical Education, Vol. 75 No. 5 May 1998

12. Analytical Chemistry for Technicians, John Kenkel, Third Edition, CRC Press LLC, 2003.

Semester II

Course Name: Physical Chemistry - II	Course Code: MSIC-201
Credit 4	**Core Course -5**

Course Objectives

1. To familiarise students with theoretical and mathematical aspects of quantised energy levels of particle in box,
2. To introduce the theoretical concept of Hydrogen atom and hydrogen molecule and hydrogen molecule ion.
3. To infer the concept of Charge on colloids, electro kinetic phenomenon's and different theories on colloids.
4. To prioritise the surface phenomenon's and different equations and theories to explain them.
5. To describe equilibrium processes of one and more than one component systems such as congruent, Peritectic and Monotectic Systems.

Course Outcomes

CO1:The concepts of quantum mechanics and its mathematical interpretation for atoms and molecules possessing single electron.
CO2: The results and their analysis obtained on the basis of MOT and VBT for hydrogen atom, molecule and ion.
CO3:The nomenclature of particles on the basis of particle size and different theories and results related to stability of colloids.
CO4: The concept of surface tension, micellization and solubilisation.
CO5: The concept of existence of different phases with change in different variables by visualizing the phase diagrams
CO6: The concept of quantum mechanics, their application to MOT and VBT, how to draw phase diagrams and importance of colloids and surface chemistry in daily life, their concepts, phenomenon and mathematical equations.

Course Description

Concept of Quantum mechanics and its applications in MOT and VBT were shared with students. Theories of colloids and concepts of surface chemistry were discussed. The phase diagram of different component systems were discussed and explained how to plot them

Outline syllabus

Unit 1 Quantum Mechanics

Matter waves, The Uncertainty principle, the wave nature of the electron, Postulates of Quantum Mechanics, Commutation of operators, Eigen value and Eigen function. Angular momentum operator, Ladder operator. The wave equation, Particle in one dimensional box, particle in three-dimensional box, Degeneracy.

Hydrogen atom: Schrodinger wave equation, Transformation of coordinates, separation of variable in polar spherical coordinates and its solution, probability distribution function, radial distribution function.

Unit 2 Chemical Bonding

Born Oppenheimer Approximation, The variation method, Ground state energy of the hydrogen atom.
Huckel molecular orbital theory of conjugated systems, Secular equations, delocalisation energy,
MOT and Valence bond theory- Hydrogen molecule.

Unit 3 Colloids

Introduction, Origin of the charges, electro-kinetic phenomena : electrophoresis, electro osmosis, sedimentation and streaming potential.
The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates.

Unit 4 Surface Chemistry and Micelles

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation.
Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm. Micelles-Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, micro emulsions, reverse micelles.

Unit 5 Phase Equilibria

Statement and meaning of the terms in Gibbs phase rule; phase equilibria of water, Helium and Carbon systems;
Two component solid-liquid equilibria (example of Cu-Ni alloy, Bi - Cd system and $CuSO_4$ – H_2O System):
simple eutectic; congruent melting type; peritectic type and monotectic type phase diagrams, concept of Phase equilibria of three component systems.

Reference Books:

1.Atkins P. W., Physical Chemistry, Oxford University Press, New York.
2.Levine I. N., Physical Chemistry, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
3 Adamson A. W., Physical Chemistry of Surfaces, John Wiley and Sons. Other References 1. Day M. C. and Selbin J., Theoretical Inorganic Chemistry. 2. Pashley R. M. and Karaman M. E., Applied Colloid and Surface Chemistry, Wiley Publications.

Semester II

Course Name: Inorganic Chemistry - II	**Course Code: MSIC-202**
Credit 4	**Core Course -6**

Course Objectives

1.To introduce the basics concept of molecular symmetry and group theory.
2.To demonstrate the various application of group theory in spectroscopy.
3.To provide an introduction to basic concepts of Organometallic chemistry.
4.To explain to the student the various application of Organometallic chemistry in industry.
5.To provide information various industrially important Organometallic compounds.
6.To provide structure, bonding and reactivity of transition metal carbonyls, nitrosyls and phosphine complexes.

Course Outcomes

CO1:Understand the various basics concept of molecular symmetry and group theory.
CO2: Apply their knowledge of group theory to understand the principles of spectroscopy.
CO3:Know the basic concepts of organometallic chemistry and its application in industry.
CO4: Explain the structure and reactivity of transition metal alkyl, aryl, alkene, alkynes, allyls, dienyl and arene and carbine complexes.
CO5: Gain insight about transition metal carbonyls, nitrosyls and phosphin complexes.
CO6: Gain knowledge about advanced topics like organometallic chemistry and group theory.

Course Description

The course includes the basic concept of group theory and its application in chemistry; as well as organometallic chemistry of transition metals.

Outline syllabus

Unit 1 Molecular symmetry

Introduction, Meaning and examples of different symmetry elements and generated operations; and general rules, Derivation of matrices for rotation; reflection; rotation; reflection and inversion operations.

Symmetry operations of all the molecular point groups (Cn, Dn, Cnh, Dnb,Cnv, Dnd, Sn, T, Td and Th .

Determination of the classes of operations by similarity transform method (only C2v, C2h, C3v) and general rules Defining properties of 'group'; Types of groups, Subgroups; reducible and irreducible representations.

Unit 2 Application of Group Theory

Construction of character table for C2v and C3v point groups.
Optical activity and dipole moment of molecules.
Applications of group theory to electronic and vibrational spectroscopy.

Unit 3 Organometallic Chemistry-I

General Characteristics of organometallic compounds, Ligand hapticity, electron count for different types of organometallic compounds, 16 and 18 electron rule and exceptions, Fluxionality in organometallic complexes.

Synthesis, structure and bonding of organolithium compounds.

Organometallic reagents in homogeneous catalytic reactions (Hydrogenation, hydroformylation, isomerisation, polymerisation).

Unit 4 Organometallic Chemistry-II

General synthetic routes, nature of bond and structural characteristics of alkyl, aryl, alkene alkynes complexes of transition metals.

Structure and bonding of metallocenes.

Synthesis, structure and reactivity of metal carbene and carbynes

Unit 5 Organometallic Chemistry-III

Ligand behavior of CO, General methods of preparation, structures, bonding, and vibrational spectra of metal (Fe, Ru, Os, Cr, Ni) carbonyls.

Ligand behavior of NO (NO^+, NO and bridging NO), preparation, structures, bonding of nitrosyls of Cr, Fe and Ru.

Preparation, structure, bonding and reactivity of metal phosphines. Comparison of phosphine and carbonyl ligands in terms of bonding.

Reference Books:

1. Inorganic Chemistry, J.E. Huhey, Harper & Row.
2. Organometallic Chemistry, R.C.Mehrotra and A.Singh, New Age International. Other References
3. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley
4. Introduction to Ligand fields, B.N. Figgis, Wiley, New York.
5. The Organometallic Chemistry of the Transit ion Metals, R.H. Crabtree, John Wiley.
6. Transition metal chemistry, Fundamental concept and applications, A.Yamamoto, John Wiley, 1986.

Semester II

Course Name: Organic Chemistry - II	**Course Code: MSIC-203**
Credit 4	**Core Course -7**

Course Objectives

This course aims to:

1. Develop an in-depth understanding of single bond (C- C) formation strategies and explore the role of enolates, enamines, and organometallic reagents in organic synthesis.
2. Develop the critical thinking to analyze the conditions required for C=C bond formation
3. Introduce metal-catalyzed carbon- carbon bond formation techniques and their applications.
4. Examine oxidation and reduction reactions, including stereochemical aspects and selectivity.
5. Analyze key name reactions and molecular rearrangements in organic synthesis

Course Outcomes

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

CO1: Utilize enolates, enamines, and organometallic reagents and metal-catalyzed coupling reactions for C- C bond formation.
CO2: Differentiate between elimination strategies for double bond formation and apply them effectively.
CO3: Implement oxidation techniques in organic synthesis with a focus on selectivity.
CO4: Understand the functional mode of various reducing reagents
CO5: Understand and predict the mechanisms of key organic name reactions and rearrangements.
CO6: Design synthetic routes using advanced organic transformations for target molecules

Course Description

This course provides a comprehensive understanding of modern organic synthesis, focusing on carbon-carbon (C-C) and carbon-carbon double bond (C=C) formation strategies. It covers the chemistry of enolates, enamines, and organometallic reagents, along with metal-catalyzed coupling reactions such as Suzuki, Heck, and Sonogashira. Key oxidation and reduction methodologies, including stereoselective transformations, are explored in detail. Additionally, the course examines important name reactions and molecular rearrangements, emphasizing their mechanisms and applications in organic synthesis. By integrating theoretical knowledge with practical applications, this course prepares students for advanced research and industrial challenges in organic chemistry.

Outline syllabus

Unit 1 Aliphatic Nucleophilic Substitution

The SN2, SN1, mixed SN1 and SET mechanism. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and non classical carbocations,

Phenonium ions, nonbornyl system, Common carbocations rearrangements. The SNi mechanism, Nucleophilic substitution at an allylic, alipahatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium.

Unit 2 Double bond (C=C) formations

Elimination reactions: Hoffmann vs. Saytzev's rule, Cope elimination, Phospohorus, nitrogen and sulfur ylides, Wittig reaction, Wittig-Horner reaction.

Mechanistic and stereochemical aspects of addition reactions involving electrophiles nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction.
Addition of Grignard reagents, Wittig reaction Mechanism of condensation reactions involving enolates–Aldol. Knoevenagel, Claisen, Mannich, Benzoin, Perkin reactions.

Unit 3 Aromatic Electrophilic Substitution

The arenium ion mechanism. orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction Gattermann-Koch reaction. Aromatic Nucleophilic Substitution The SNAr. SN1 . benzene and SRN 1 mechanisms. Reactivity - effect of substrate structure. leaving group and attacking nucleophile. The von Richter. Sommelet-Hauser and Smiles rearrangements.

Unit 4 Oxidation and Reduction

Alkene oxidation: alkenes to carbonyls with bond cleavage, alkenes to alcohols/carbonyls without bond cleavage (Wacker oxidation).
Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification.
Oxidation of Alcohols: alcohols to carbonyls, alcohols to acids or esters, phenols (Fremy's salt), Swern oxidation.
Catalytic reduction (Pt, Pd, Ni), Dissolving metal reductions (alkali metals in Liq. NH_3 and Zn, Sn).

Reduction by hydride transfer reagents (Complex hydrides of Li and Na); Steroeselectivity of reduction with small hydride donors.

Reduction with non-metals: HI, Diimides and hydrazine.

Unit 5 Name Reactions and Molecular Rearrangements

A Hoffmann, Lossen, Curtius, Schmidt rearrangement
Mechanism of Baeyer Villiger, Favorskii rearrangement, Sommelet-Hauser rearrangement
Baylis-Hillman reaction, Henry reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction.

Reference Books

1. Organic Reactions and Mechanisms, P.S. Kalsi, (2002) 2nd Edition, New Age International Publishers.
2. Organic Chemistry, R. T. Morrison and R. N. Boyd, (1992) 6th Edition, Prentice-Hall.
3. Reaction Mechanism in Organic Chemistry, (1976) 1 st Edition, S. M. Mukherji and S. P. Singh, Macmillan.
4. Advanced Organic Chemistry Reactions: Mechanism and Structure, Jerry March, (1992) 4th Edition, John Wiley.
5. Organic Chemistry, Francis A. Carey, (1996) 3rd Edition, The McGraw-Hill Companies, Inc.
6. Modern Methods of Organic Synthesis South Asia Edition W. Carruthers, Iain Coldham, (2004) 4th Edition, Cambridge University Press 4. Principles of Organic Synthesis, R.O.C. Norman, (1978) 2nd Edition, Chapman and Hall.

Semester II

Course Name: Analytical Chemistry II	**Course Code: MSIC-204**
Credit 4	**Core Course -8**

Course Objectives

1. Understand the theories and principles of qualitative and quantitative analysis through optical and spectroscopic technique.
2. Analyse the textural information of bulk materials and particle dimension.
3.Carry out qualitative and quantitative analysis employing descriptive knowledge of electrochemistry and electrochemical titration.
4.Separate and estimate macromolecule (proteins, enzymes, blood and natural products) electroanalytically.
5.Effectively use various sensors for estimation and gain idea about developing technologically potent sensor materials.
6. To learn the advance spectroscopic and microscopic methods for the analysis of molecular materials.

Course Outcomes

CO1: Understand various optical and spectroscopic methods for qualitative and quantitative analysis of metals and non- metal to trace level.
CO2: Evaluate the properties of materials such as porosity, density and microstructure of materials.
CO3: Develop new synthetic routes involving electrochemical redox process.
CO4: Understand principles of Cyclic Voltammetry and Electrophoresis.
CO5: Develop quick, sensitive and selective sensory materials for qualitative and quantitative estimation of analyte.
CO6: Investigate the molecular materials using advanced spectroscopic and microscopic techniques.

Course Description

Analytical chemistry II emphasizes on various parts of analytical methods as - Atomic Spectroscopy comprises of AAS, AES and ICPMS, Electron Microscopic techniques comprises of SEM, TEM and FESEM, Polarography and amperometry, Cyclic voltammetry and electrophoresis Chemical sensors.

Outline syllabus

Unit 1 Atomic Spectroscopy

Theory, sources, burners, atomic emission spectra, atomic absorption spectra, effect of temperature on emission

and absorption, Instrumentation for AES and AAS, standard addition and internal standard method of analysis Comparison of atomic absorption and emission methods, Applications of AAS and AES Features of atomic mass spectroscopy, Atomic weight in mass spectroscopy, mass to charge ratio
Types of atomic mass spectroscopy, quadruple mass analyzer, time of flight mass analyzer, Inductively coupled mass spectroscopy (ICPMS), Instrumentation for ICPMS, Applications of ICPMS.

Unit 2 Electron Microscopic Techniques

Basic principle, instrumentation and application of Transmission Electron Microscope (TEM) and HRTEM
Basic principle, instrumentation and application of Scanning Electron Microscope (SEM)
Basic principle, instrumentation and application of FESEM

Unit 3 Electroanalytical Technique - I

Polarography Introduction, Instrumentation, Ilkovic equation and its verification
Derivation of wave equation, Determination of half wave potential, qualitative and quantitative applications
Amperometry: Basic principles, instrumentation, nature of titration curves and analytical principles

Unit 4 Electroanalytical Technique - II

Cyclic Voltammetry Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry, interpretation of voltammograms.
Electrophoresis: Separation by adsorption-Affinity techniques, affinity elution from ion exchangers and other adsorbents.
Pseudo affinity adsorbents, polyacrylamide get electrophoresis, isoelecrictric focusing, isotachophoresis

Unit 5 Chemical Sensors

A Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials
Solid electrolyte, gas, semiconductor, Humidity sensors, Biosensors sensors.
Electrochemical sensors (Potentiometric sensors, Ionselective electrodes, Membrane electrodes, Amperometric sensors).

Reference Books:

1. Principles of Instrumental Analysis, Skkog, Holler, Nieman, (Sixth Ed.) Other References 1)
2. Introduction to Instrumental Analysis by R. D. Broun, Mc Graw Hill (1987)
3. Instrumental methods of chemical analysis by H. willard, L.Merrit, J.A. Dean and F.A. settle. Sixth edition CBS (1986)
4. Fundamentals of Analytical Chemistry, 6th edition, D.A. Skoog, D.M. West and F.J. Holler, Saunders college publishing.

5. Principles of Instrumental Analysis, Skkog, Holler, Nieman, (Sixth Ed.)
6. Introduction to instrumental analysis by R. D. Braun, MC. Graw HillInternational edition.
7. Analytical Chemistry, Ed. by Kellner, Mermet, otto, Valcarcel, Widmer, Second Ed. Wiley –VCH
8. Electron microscopy in the study of material, P. J Grundy and G. A Jones, Edward Arnold.

Semester II

Course Name: Qualitative & Quantitative Analysis of Organic Compounds	**Course Code: MSIC-205P**
Credit 4	**Practical Course -3**

Outline syllabus

Part A

1. Isolation and identification of multi-functional compounds in a mixture of two organic compounds.

2.Identification of three acidic and basic radicals in the given mixture (sample 1)

3. Identification of three acidic and basic radicals in the given mixture (sample 2)

4. Application of spectral data (IR, UV, NMR and mass) for structural elucidation

5. Isolation of natural products:

i) Isolation of caffeine from tea leaves

ii) Isolation of piperene from black pepper

iii) Isolation of β-carotene from carrots

iv) Isolation of lycopene from tomatoes

v) Isolation of limonene from lemon peel

vi) Isolation of Euginol from cloves

Part B

6. Quantitative analysis:

i) Estimation of glucose by chemical methods

ii) Estimation of amino acids by chemical methods

iii) Estimation of nitro group in organic compounds

iv) Estimation of iodine number by Vij's solution

v) Estimation of protein, caffeine and glucose by UV/VIS spectra (quantitative analysis also)

vi) Estimation of ascorbic acid by chemical/UV methods

7**. Advanced organic synthesis: Multistage synthesis including photochemical methods; representative examples:**

i) Benzophenone → benzopinacol → benzopinacolone

ii) Benzoin → benzil → benzilic acid

iii) Benzaldehyde → chalcone → chalcone epoxide

iv) Chalcone → chalcone dibromide → a-bromochalcone

v) Cyclohexanone → cyclohexanone oxime → caprolactone

Reference Books:

1.Vogel's Textbook of Practical Organic Chemistry" by B.S. Furniss et
2.Systematic Qualitative Organic Analysis" by H.T. Clarke
3.Spectrometric Identification of Organic Compounds" by Robert M. Silverstein, Francis X. Webster, David J. Kiemle
4.Practical Organic Chemistry: Preparations and Quantitative Analysis" by Mann and Saunders
5. Natural Products: A Laboratory Guide" by Raphael Ikan

Semester II

Course Name: Analytical Method Development and Validation	**Course Code: MSIC-206P**
Credit 4	**Practical course - 4**

Course Outcomes

At the end of course students should able to
1. Define / understand various chemical terms involved Method development and validation.
2. Explain statistical parameters of Method development.
3.Apply / select particular method / instrumental parameters for analysis of given sample and give mathematical treatment to analytical data and able to interpret the results accurately.
4. Analyze the results able to take the decision regarding quality of sample.
5. Maintain proper record of analytical data in notebook.
6. Design / modify and validate new analytical method for chemical analysis of particular sample.

Outline syllabus

1. **Table Work:** a) Explain with example of each Accuracy, precision, noise level, detection limit, quantitation limit, b) Explain with example: Expression of results: Calculation of mean, standard deviation, error and absolute error, significant figure; Propagation of errors c) Explain with example: Calibration curve and standard addition method, Regression analysis of calibration curve and its importance.
Calculations using EXCEL: mean,standard deviation, plotting calibration curve and equation of line, regression, axis labelling, etc.

2. Determination of Alkalinity of Natural Waters.
3. Determination of Hardness in a Water Sample
4 **Analytical method development and validation Study of visible spectroscopic or colorimetric method for estimation of particular metal ion:**

a) Determination of best pH for colour formation reaction, and determination of λmax for quantitative analysis using limited conc. of metal ion and large excess ligand;

b) Determination of metal ligand ratio at best pH. B) Detection of possible interfering metal ion (such as Ca(II), Mg(II), Mn(II), Ni(II), Co(II), Cu(II), Fe(II)).

5. Estimation of Glucose – Glucose in different samples can be analysed by
i) titration with Fehling solution
b) Colorimetry Folin-Wu method or DNSA method
c) Colorimetry-Glucose by oxidase peroxidase method and
d) Polarimetry.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Samples are –
a) glucose in saline (DNS),
b) glucose in glucose supplement
c) glucose in food. Mentor will assign any one sample to the student. Student have to choice suitable method for analysis of glucose in sample with reason. After discussion with mentor analyse the sample by particular method. .

6. Perform pH metric titration for estimation of CH3COOH from vinegar using i) 0.1 M standardized NaOH using phenolphthalein indicator ii) 0.5 M standardized NaOH using pH meter. Compare the results of two methods and give your comment.

7. Determine Paracetamol in tablet conventional titration (redox titration with Ceric ammonium nitrate) and by potentiometric titration (redox titration using Pt and Calomel electrode) and compare the results of two method.

8. Benedict's test to determine the presence of reducing sugar.

9. Fehling's test to determine the presence of reducing sugar.

10. Iodine test to distinguish starch from other polysaccharides.

11. Molisch's test for detection of Monosacchrides.

Reference Books:

1. Separation, Preconcentration and Spectrophotometry in Inorganic Analysis, by Z. Marczenko and M. Balcerzak, Analytical Spectroscopy Library – 10, Elsevier
2. Standard methods for the examination of water and wastewater, 23rd Ed. Roger B. Baird, Andrew D Eaton, Eugene W. Rice, American Public Health Association, Americal water works association, Water environment federation.
3. Vogels textbook of Inorganic Quantitative Analysis, 6 th Ed, Pearson
4. Biochemical Methods, Third Edition, By S Sadashivan, A. Manickam; New Age International Publishers
5. Indian Pharmacopeia: 2007, Vol-1, 2, 3.
6. Chemical Analysis and Material Characterization by spectrophotometry, Bhim Prasad Kafle, Elsevier
7.. Ultraviolet and Visible Spectrophotometry in Pharmaceutical Analysis, Sandor Gorog, Published by CRC press, Taylor and Fransis.
8. An introduction to Practical Bichemistry, David T. Plummer, Tata McGraw-Hill publishing Company Ltd.
9. Manual Of Methods Of Analysis Of Foods Food Safety And Standards Authority Of India Ministry Of Health And Family Welfare Government Of India New Delhi 2015
10. Food Analysis, Edited by S. Suzanne Nielsen, Fourth Edition, Springer.

Semester II

Course Name: Intellectual Property Rights	Course Code: CHM
Credit 2	

Unit I Overview of Intellectual Property

Introduction and the need for intellectual property right (IPR). IPR in India – Genesis and Development IPR in abroad. Some important examples of IPR.

Unit II Patents

Macro economic impact of the patent system. Patent and kind of inventions protected by a patent. Patent document. Protection of inventions. Granting of patent. Rights of a patent. Patent protection. Protection of inventions by patents. Searching, Drafting and Filing of a patent. The different layers of the international patent system (national, regional and international options).

Unit III: Patents: Utility models

Differences between a utility model and a patent. Trade secrets and know-how agreements.
Copyright: Introduction, How to obtain, Differences from Patents. Related rights. Distinction between related rights and copyright. Rights covered by copyright.

Unit IV Trademarks

Trademark, Rights of trademark. Kind of signs used as trademarks. Types of trademark. Function does a trademark perform. Protection and registration of trademark. Duration of trademark protection. Well-known marks and their protection. Domain name and it relate to trademarks.

Unit V Industrial Designs

Industrial design. Protection of industrial designs. Kind of protection is provided by industrial designs. Duration of protection.
IP Infringement issue and enforcement – Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Intellectual Property in the Indian Context – Various laws in India Licensing and technology transfer.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Reference Books

1. Ajit Parulekar and Sarita D' Souza, Indian Patents Law – Legal & Business Implications; Macmillan India ltd, 2006
2. B.L.Wadehra; Law Relating to Patents, Trade Marks, Copyright, Designs & Geographical Indications; Universal law Publishing Pvt. Ltd., India 2000
3. P. Narayanan; Law of Copyright and Industrial Designs;Eastern law House, Delhi , 2010
4. N.K. Acharya: Textbook on intellectual property rights, Asia Law House (2001).
5. Manjula Guru & M.B. Rao, Understanding Trips: Managing Knowledge in Developing Countries, Sage Publications (2003).
6. P. Ganguli, Intellectual Property Rights: Unleashing the Knowledge Economy, Tata McGraw-Hill (2001).

Course Name -M. Sc. Industrial Chemistry													
Batch:2025-27								SEMESTER:III					
S. No.	Course Type	Course Code	Course Name	Teaching Load			Credits	Internal Assessment				External Assessment	Total
				L	T	P							
THEORY and PRACTICAL SUBJECTS								CLASS PARTICIPATION	Quiz/PPT/Assignment (10)	Mid Sem Test (15)	TOTAL	End Sem Exam (70)	
1	CORE COURSE-9	MSIC-301	Chemistry of Agro Chemicals, Textiles and Polymers	4	0	0	4	5	10	15	30	70	100
2	CORE COURSE-10	MSIC-302	Chemistry of Industrial Minerals	4	0	0	4	5	10	15	30	70	100
3	DISCIPLINE ELECTIVE COURSE -1	MSIC-303A/MSIC-303B/MSIC-303C/MSIC-303D	Bioinorganic Chemistry/Bioorganic Chemistry/Biophysical Chemistry/Natural Products Chemistry	4	0	0	4	5	10	15	30	70	100
4	DISCIPLINE ELECTIVE COURSE -2	MSIC-304A/MSIC-304B/MSIC-304C/MSIC-304D	Nanochemistry/ Organometallic Chemistry/ Quantum Chemistry/ Surface Chemistry	4	0	0	4	5	10	15	30	70	100
5	PRACTICAL COURSE- 5	MSIC-305P	Industrial Chemistry Laboratory -1	0	0	8	4	5	10	15	30	70	100
6	PRACTICAL COURSE-6	MSIC-306P	Industrial Chemistry Laboratory -2	0	0	8	4	5	10	15	30	70	100
7	OEC		To Be selected from the Bucket of Courses	2	0	0	2	4	4	7	15	35	50
TOTAL CREDITS / ASSESSMENT							**26**	34	64	97	195	455	**650**

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

KERAL VERMA SUBHARTI COLLEGE OF SCIENCE

Course Name -M.Sc. Industrial Chemistry

Batch:2025-27 — **SEMESTER:IV**

S. No.	Course Type	Course Code	Course Name	Teaching Load L	T	P	Credits	Internal Assessment: CLASS PARTICIPATION	Quiz/PPT/Assignment (10)	Mid Sem Test (15)	TOTAL	External Assessment: End Sem Exam (70)	Total
THEORY and PRACTICAL SUBJECTS													
1	CORE COURSE -11	MSIC-401	Pharmaceutical Chemistry	4	0	0	4	5	10	15	30	70	100
3	DISCIPLINE ELECTIVE COURSE -3	MSIC-402A/MSI-402B/MSIC 402C/MSIC 402D	Green Chemistry/ Polymer Chemistry/ Material Chemistry/Computational Chemistry	4	0	0	4	5	10	15	30	70	100
4	DISCIPLINE ELECTIVE COURSE -4	MSIC-403A/MSIC 403B/MSIC 403C/MSIC -403D	Medicinal Chemistry/ Environmental Chemistry/ Photochemistry/ Supramolecular Chemistry	4	0	0	4	5	10	15	30	70	100
5	DISSERTATION	MSIC-404	Project	4	0	8	12	20	30	50	100	200	300
7	EEC			0	0	0	2	4	4	7	15	35	50
TOTAL CREDITS / ASSESSMENT							26	39	64	102	205	445	650

Course Name -M.Sc. Industrial Chemistry

Batch:2025-27 — **SEMESTER:IV**

S.No.	Course Type	Course Code	Course Name	Teaching Load L	T	P	Credits	Internal Assessment: CLASS PARTICIPATION	Quiz/PPT/Assignment (10)	Mid Sem Test (15)	TOTAL	External Assessment: End Sem Exam (70)	Total	Remark
THEORY and PRACTICAL SUBJECTS														
1	DISSERTATION	PC-1	Project	4	0	8	26	20					650	
TOTAL CREDITS / ASSESSMENT														

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Semester - III

Course Name: Chemistry of Agrochemicals, Textiles and Polymers	**Course Code: MSIC-301**
Credit 4	**Core Course -9**

Course Objectives

1. Explain the chemistry, mode of action, and industrial significance of major classes of agrochemicals including fertilizers, insecticides, herbicides, fungicides, and plant growth regulators.
2. Familiarize students with textile fiber chemistry, dyeing techniques, finishing processes, and the role of various auxiliaries and chemicals used in textile industries.
3. Provide knowledge on polymer chemistry, including mechanisms of polymerization, classification, synthesis, molecular weights, and structure–property relationships.
4. Introduce industrial manufacturing processes, quality control methods, and performance evaluation techniques for agrochemicals, textiles, and polymers.
5. Develop awareness about environmental impacts, green chemistry alternatives, regulatory standards, and safe handling of chemical products.
6. Equip students with problem-solving and analytical skills relevant to research, testing, and industrial applications in agrochemical, polymer, and textile sectors.

Course Outcomes

CO1: Demonstrate knowledge of pesticides, herbicides, fungicides, and fertilizers, including their synthesis, mode of action, and environmental behavior**.**

CO2: Explain industrial production methods, formulation chemistry, toxicology, and regulatory standards for safe agrochemical usage.

CO3: Analyze the chemical composition of natural & synthetic fibers and describe dyeing, bleaching, scouring, and textile finishing operations**.**

CO4: Identify chemicals used in sizing, printing, finishing, and understand the chemistry behind color development and fastness properties.

CO5: Explain mechanisms of polymerization, molecular weight determination, polymer characterization techniques, and structure–property relationships.

Course Description

This course provides an in-depth understanding of the chemical principles, synthesis, properties, and industrial applications of agrochemicals, textile chemicals, and polymers. It covers the chemistry and formulation of fertilizers, pesticides, herbicides, and growth regulators; the processing and finishing of textile fibers; and the classification, polymerization techniques, properties, and applications of synthetic and natural polymers. The course emphasizes industrial production methods, environmental and safety aspects, quality control, and recent advancements such as green chemistry, biodegradable polymers, and sustainable agrochemical practices.

Outlined syllabus

Unit 1 Chemistry of Agrochemicals

Introduction, role of agrochemicals in agriculture, classification of agrochemicals; Pesticides: Classification, general synthesis, chemical structure, mode of action, and toxicity of various insecticides, herbicides, and fungicides (e.g., organophosphates, carbamates, triazines). Fertilizers: Chemistry of nitrogenous, phosphatic, and potassic fertilizers; manufacturing processes (e.g., ammonia, urea, superphosphate); controlled-release fertilizers.

Safety and Regulations: Environmental impact, pollution control, and regulatory standards for agrochemicals.

Unit 2 Chemistry of Textiles

Fiber Chemistry: Chemical structure, properties, and manufacturing of natural (cotton, wool, silk) and synthetic fibers (polyester, nylon, acrylic, rayon).

Dyeing and Printing: Classification, chemistry, and application methods of various dyes (e.g., azo dyes, vat dyes, reactive dyes); principles of color and dyeing machinery.

Textile Processing: Chemistry of pre-treatment (scouring, bleaching, mercerization) and finishing (softening, fire-retardant, wrinkle-free) chemicals.

Unit 3 Chemistry of Polymers

Polymers Fundamentals: Classification, nomenclature, molecular weight determination methods, and thermal properties (e.g., glass transition temperature, T_g).

Polymerization: Detailed mechanism and kinetics of various techniques: addition (free radical, ionic, coordination) and condensation polymerization.

Industrial Polymers: Synthesis, properties, and applications of major thermoplastics (PE, PP, PVC, PS) and thermosets (epoxy, phenolic resins), and elastomers (synthetic rubbers).

Polymer Technology: Compounding, processing techniques (injection molding, extrusion), and polymer degradation.

Reference Books

1. K.H. Buchel, Chemistry of Pesticides, Wiley–VCH.
2. A.L. Banerjee, Agrochemicals and Pesticides, Oxford & IBH Publishing.
3. E.P.G. Gohl & L.D. Vilensky, Textile Science, CBS Publishers.
4. S.R. Karmakar, Chemical Technology in the Pre-Treatment Processes of Textiles, Elsevier.
5. F.W. Billmeyer, Textbook of Polymer Science, Wiley India.

Semester - III

Course Name: Chemistry of Industrial Minerals	**Course Code: MSIC -302**
Credit 4	**Core Course - 10**

Course Objectives

1. Understand the chemistry and mineralogy of key industrial minerals including silicates, carbonates, sulfates, clays, phosphates, and metallic ores.
2. Explain the relationship between crystal structure, chemical composition, and physical properties of industrial minerals.
3. Evaluate industrial applications of minerals based on their chemical behavior and functional properties.
4. Describe processing and beneficiation techniques, including thermal, chemical, and mechanical methods used in mineral industries.
5. Assess environmental, sustainability, and economic considerations in the extraction, processing, and utilization of industrial minerals.

Course Outcome

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

CO1: Identify and classify major industrial minerals based on their chemical composition and mineralogical structures.
CO2: Analyze the physicochemical properties of industrial minerals and correlate them with their industrial uses.
CO3: Explain the chemical reactions and transformations involved in mineral processing techniques such as calcination, leaching, flotation, and roasting.
CO4: Perform basic mineral characterization using standard analytical tools and interpret the resulting data.
CO5: Evaluate the suitability of specific minerals for applications in cement, ceramics, metallurgy, polymers, electronics, agriculture, and environmental systems

Course Description

This course introduces the chemical principles, mineralogical characteristics, industrial applications, and processing technologies of major industrial minerals. Students will learn analytical techniques used to characterize industrial minerals and understand chemical modifications that enhance their performance in industrial processes. The course integrates theoretical foundations with real-world case studies relevant to mineral-based industries.

Outline syllabus

Unit 1 Introduction to Industrial Minerals

Introduction, scope, and economic importance, classification and Occurrence: Major industrial minerals (e.g., silicates, carbonates, phosphates, sulfides) and their geological distribution.

Processing: Principles of beneficiation, froth flotation, magnetic and gravity separation, and particle size reduction. Overview of world reserves and distribution and their role in modern industries.

Unit 2 Specific Mineral-Based Industries

Cement and Ceramics: Chemistry of Portland cement manufacturing (clinkering, setting, hardening); traditional and advanced ceramics (e.g., refractories, structural ceramics, porcelain).

Glass and Silicates: Chemistry of glass formation, types of glasses (soda-lime, borosilicate), and manufacturing processes; chemistry of various silicates (e.g., zeolites, asbestos).

Metallurgy: Principles of pyrometallurgy (smelting, refining), hydrometallurgy (leaching, solvent extraction), and electrometallurgy for extracting metals like copper, aluminum, iron, and zinc.

Pulp and Paper: Chemistry of wood components (cellulose, lignin), pulping processes (kraft, sulfite), bleaching, and paper additives.

Industrial Gases: Production and applications of industrial gases like oxygen, nitrogen, hydrogen, and acetylene.

Unit 3 Basic theory, instrumentation and analytical applications of the following techniques

Powder X-Ray Diffraction (PXRD), structure determination from PXRD, phase identification, and crystallite size determination.
Electron Microscopy: Principles and application of scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive analysis of X-rays (EDAX).

Surface Characterization Techniques: X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), ESCA and their applications. Brunauer-Emmett-Teller (BET) surface area analysis and adsorption isotherms, temperature programmed desorption (TPD), temperature programmed oxidation (TPO) and temperature programmed reduction (TPR), zeta-potential measurements.

Electrical properties: Polarography; cyclic voltammetry; chrono-methods; AC impedance techniques - concepts and applications

Reference Books

1. J. W. Anthony, Industrial Minerals: Their Composition, Properties, and Uses, Wiley.
2. A. Gupta, D.S. Yan, Mineral Processing Design and Operations: An Introduction, Elsevier.
3. S.C. Misra, Principles of Mineral Processing, CBS Publishers.
4. C.J. Brinker, G.W. Scherer, Sol-Gel Science: The Physics and Chemistry of Sol-Gel Processing, Academic Press.
5. W.D. Callister, Materials Science and Engineering: An Introduction, Wiley.
6. J. Paul, Pulp and Paper Chemistry and Technology, TAPPI Press.
7. P. O’Connor, P. Sexton, R. Smart, Surface Analysis Methods in Materials Science, Springer.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Semester - III

Course Name: Bioinorganic Chemistry/ Binorganic Chemistry/ Biophysical Chemistry/ Natural Products	**Course Code: MSIC-303A/ MSIC-303B/ MSIC-303C/ MSIC-303D**
Credit 4	**Discipline Elective course - 1**

Bioinorganic Chemistry

Course Objectives

1. To describe about basic principles and importance of various metals in natural systems.
2. To describe various ion transport through biological membrane.
3. To explain the importance of Iron and Copper containing metallo-biomolecule.
4. To illustrate the chemistry of bio molecules like DNA and RNA.
5. To describe the bioinorganic chemistry of Molybdenum, Tungsten and Zinc containing Enzymes.
6. To describe the bioinorganic chemistry of Vitamin B12.
7. To describe the bioorganic chemistry of enzymes and Co-enzymes.
8. To describe the biophysical chemistry of biopolymers and their molecular weights.

Course Outcome

CO1: Explain the transport of ions through membrane
CO2: Predict the structure and mechanism of Fe and Cu containing metalloproteins.
CO3: Learn about structure and chemistry of DNA and RNA.
CO4: Understand the importance of Molybdenum, Tungsten and Zinc containing Enzymes.
CO5: Illustrate biologically important processes like photosynthesis
CO6: Understand the role and importance of metal ions in biology.
CO7: Explain the role of enzyme and co enzyme in reactions.
CO8: Learn about biopolymers and their molecular weights.

Course Description

This course includes details discussion about various bio molecules and metal containing enzymes with special reference to iron, copper, zinc, tungsten and molybdenum.

Outline syllabus

Unit 1 Bioinorganic Chemistry of Metals

Essential and trace elements in biological systems,
structure and functions of biological membranes; mechanism of ion transport across membranes; sodium pump,
Role of calcium in blood clotting
Structure and functions of amino acids, proteins, peptides

Unit 2 Bioinorganic Chemistry of Iron and Copper

Iron-sulphur proteins: rubredoxin and ferredoxins;
Heme proteins: hemoglobin, myoglobin. Cytochrome P-450, Cytochrome c-oxidase and cytochrome
Synthetic oxygen carrier and model systems. Nonheme proteins: hemerythrin and hemocyanin.

Unit 3 Bioinorganic Chemistry in Biological Systems

A Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA and RNA).

Stability of DNA and melting temperature.
Role of metal ions in replication and transcription process of nucleic acids.

Unit 4 Molybdenum, Tungsten and Zinc containing Enzymes

Enzymes and their classification; Importance of Zn in nature, carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase.

Biological nitrogen fixation (Nitrogenase) and abiological nitrogen fixation

Tungsten containing formate dehydrogenase and tungsten bearing hyperthermophilic enzymes.

Unit 5 Biologically Important Processes

Photosynthetic electron transport chain,
chlorophyll, PS-I and PS-II, Vitamin B 12 coenzyme, its function
Availability of iron and iron toxicity.

Reference Books

1. S. J. Lippard & J. M. Berg. Principles of Bioorganic Chemistry; Panima Publ. Corpn. (2005).
2. E. -I. Ochiai. Bioinorganic Chemistry; An Introduction; Allyn and Bacon Inc. (1977). Other References 1.M. N. Hughes. The Inorganic Chemistry of Biological Processes; Wiley (1981).
3.R. P. Hanzlik. Inorganic Aspects of Biological and Organic Chemistry; Academic Press (1976).
4.H. Kraatz & N. Metzler-Nolte (Eds.). Concepts and Models in Bioinorganic Chemistry; Wiley (2006).
5.Bertini; H. B. Gray; S. J. Dippard & J. S. Valentine; Bioinorganic Chemistry; Viva Books Pvt. Ltd. (2004).
6.A. W. Addison; W.R. Cullen; D. Dolphin & B.R. James (eds.). Biological Aspects of Inorganic Chemistry; John Wiley (1977).

<u>Bioorganic Chemistry</u>

Unit 1 Enzymes & Mechanism of Enzyme

Action Introduction and historical perspective, chemical and biological catalysis, properties of enzymescatalytic power, specificity and regulation. Fischer’s lock and Koshland’s induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed, mutagenesis. Enzyme kinetics, Michaelis-Menten and LineweaverBurk plots, reversible and irreversible inhibition. Transition-state theory, acid-base catalysis, covalent catalysis, strain of distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Unit 2 Kinds of Reactions Catalysed by Enzymes

Nucleophillic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and -cleavage andβelimination reactions, enolic intermediates in isomerization reactions, condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Unit 3 Co-Enzyme Chemistry

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+ , NADP+ , FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

Unit 4 Enzyme Models

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyxlodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.

Unit 5 Biotechnological Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, use of enzymes in food and drink industry, brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Unit 6 Biological Cell and its Constituents

Cell Membrane and Transport of Ions Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Structure and functions of cell membrane, ion transport through cell membrane. II. Bioenergetics Standard free energy change in biological reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Biophysical Chemistry

Unit 1 Biological Cell and its Constituents

Cell Membrane and Transport of Ions Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition. Structure and functions of cell membrane, ion transport through cell membrane.

Unit 2 Bioenergetics

Standard free energy change in biological reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Unit 3 Statistical Mechanism in Biopolymers

Chain configuration of macromolecules, statistical distribution, end-to-end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

Unit 4 Biopolymer Interactions

Thermodynamics of Biopolymer Solutions Forces involved in biopolymer interactions. Electrostatic charge and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

Unit 5 Biopolymers and their Molecular Weights

Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions

Reference Books for Bioinorganic Chemistry / Bioorganic Chemistry / Biophysical Chemistry

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
4. Understanding Enzymes, Trevor Palmer, Prentice Hall.

5. Enzyme Chemistry: Impact and Applications, Ed. Colliins J Sucking, Chapman and Hall.
6. Enzymes Mechanism Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
7. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
8. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
9. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman.
10. Enzymatic Structure and Mechanism, W.H. Freeman.
11. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
12. Biochemistry, L. Stryer, W.H. Freeman. 13. Biochemisty, J. David Rawn, Neil Patterson.
13. Biochemistry, Voet and Voet, John Wiley.
14. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
15. Macromolecules: Structure and function, F. World, Prentice Hall.

Natural Products Chemistry

Unit 1 Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure, determination, isoprene rule, Structure determination, stereochemistry biosynthesis and synthesis of the following representative molecules : Citral, Geraniol,α termpeneol Menthol, Farnesol, Zingiberen.

Unit 2 Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods or structure elucidation, degradation, classification based on nitrogen heterocyclic rings, role of alkaloids in plants, Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+) Coniline, Nicoline, Atropine, Quinine and Morphine.

Unit 3 Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholestrol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone, Biosynthesis of steroids.

Unit 4 Plant Pigments

Occurrence, nomenclature and general methods of structure determination, Isolation and synthesis of Apigenin, Luteolin, Quercetin, mytcelin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin -7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Unit 5 Prophyrins

Structure and synthesis of Haemoglobin and Chlorophyll.
Prostaglandins
Occurrence, biogenesis and physiological effects Synthesis of PGE2 and PGF2

Reference Books

1. Finar, I. L. Organic Chemistry (Volume 2: StereoChemistry and the Chemistry of Natural Products),Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiParakashan (2010).

Semester - III

Course Name: Nanochemistry / Organometallic Chemistry/ Quantum Chemistry/ Surface Chemistry	**Course Code: MSIC-304A/ MSIC-304B/ MSIC-304C/ MSIC-304D**
Credit 4	**Discipline Elective course - 2**

Nanochemistry

Unit 1 Fundamentals of Nanotechnology

Introduction to Nano-science and Nano-technology, Nano-scale material, implications for Physics, Chemistry, Engineering & Biology, and Motivation for Nanotechnology study. History & development of Nano-science and Nano-technology with the emphasis on history of Nano-metals, Chalcogenides& Boron Nitrite and Carbon Nanomaterials

Unit 2 Structures & Classification of Nanomaterials

Nano-structures: various types of nano-structures and nano-crystals. Classification: of bulk Nanostructured materials, 0D, 1D, 2D structures – Size Effects – Fraction of Surface Atoms – specific Surface Energy and Surface Stress – Effect on the Lattice Parameter – Phonon Density of States Nano-particles, Quantum dots, Nano-wires, Ultra-thin films, Multi-layered materials.

Unit 3 Nanomaterials

Introduction: Properties of materials & nanomaterials, role of size and shape in nanomaterials. Electronic Properties: Classification of materials: Metal, Semiconductor, Insulator, Band structures, Brillouin zones, Mobility, Resistivity. Magnetic Properties: Superparamagnetism, blocking. Important properties in relation to nanomagnetism.
Optical Properties: Photoconductivity, Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence. Thermal Properties and Mechanical Properties;

Unit 4 Synthesis and Characterization of Nanomaterials

Chemical Methods: Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Post-synthetic size-selective processing. Solgel, Micelles and microemulsions.

Biological Methods of Synthesis: Use of bacteria, fungi, Actinomycetes for nanoparticles synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Viruses as components for the formation of nanostructured materials; Synthesis process and application, Role of plants in nanoparticle synthesis.

Characterization Techniques: X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR Spectrophotometers

Reference Books

1. C. Bre´chignac P. Houdy M. Lahmani, Nanomaterials and Nanochemistry, Springer Berlin Heidelberg, Germany (2006).
2. Kenneth J. Klabunde, Nanscale materials in chemistryлђ, Wiley Interscience Publications (2001).
3. Hans Lautenshlager, Emulsionsлђ, Kosmetik International, (2002).
4. Roque Hidalgo-Alvarez, Structure and Functional properties of Colloidsлђ, CRC Press, (2009).
5. Richard J. Fann, Chemistry and Technology of Surfactantsлђ, Wiley-Blackwell, (2006)

Organometallic Chemistry

Unit 1 Alkyls and Aryls of Transition Metals

Alkyls and aryls of transition metals, nature of metal carbon bond, routes of synthesis, stability and decomposition pathways and their structure. Alkyls and aryls of s-block and p-block elements. Comparison of such transition and non-transition element derivatives. Organocopper in organic synthesis.

Unit 2 Compounds of Transition metal-carbon multiple bonds

Alkylidenes, alkylydines, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit 3 Transition Metal π-Complexes

Transition Metal π-Complexes with unsaturated organic molecules. Alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes; preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit 4 Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

Unit 5 Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as $\eta2$ -olefin, $\eta3$ -allyl and dienyl complexes, their characterization.

Reference Books

1. Principle and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.P. Norton and R.G. Finke. University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh; New Age International.

Quantum Chemistry

Unit 1 Quantum Mechanics

Matter waves, The Uncertainty principle, the wave nature of the electron, Postulates of Quantum Mechanics, Commutation of operators, Eigen value and Eigen function. Angular momentum operator, Ladder operator.
The wave equation, Particle in one dimensional box, particle in three-dimensional box, Degeneracy.
Hydrogen atom: Schrodinger wave equation, Transformation of coordinates, separation of variable in polar spherical coordinates and its solution, probability distribution function, radial distribution function.

Unit 2 Prerequisite

Legendre, associated Legendre polynomials; Hermite polynomials; Lagurre and associated Lagurre polynomials; polynomials as orthonormal functions, their properties; step-up and step-down operators, application to single electron and multi-electron atom, eigen-ket-ladder and formulation of spherical harmonics from angular momentum rules, finite rotation operation vs. angular momentum operators, spin angular momentum, Pauli spin matrices — spin eigenfunctions and their properties. coupling of angular momentum for many electron system, spin-orbit coupling, Molecular term symbols. Quantum tunnel effect. Fermi and Bose gases.

Unit 3 Approximate methods

A Time dependent perturbation theory, semi classical treatment of radiation-matter interaction, transition probability and rates, Einstein's A and B coefficients, selection rules; Oscillator strength,
Variation theorem and variational methods: principles of linear and non-linear variation methods,
stationary perturbation theory for non-degenerate and degenerate states - applications to rotator, Stark effect.

Unit 4 Many electron systems

An Antisymmetry of many electron wave function, spin and spatial orbitals, Slater dESErminant; closed-shell and open-shell electron configurations; multi-electron purespin state wave functions - examples with 2- and 3-electron systems, formulation of a multi-electron closed-shell electron configuration energy, introduction of core, Coulomb and exchange integrals with their properties - example of He atom, independent particle model, multi-electron atomic Hartree Hamiltonian and related SCF equations solution, Roothaan-Hartree-Fock method vertical ionization potential and Koopman's theorem; Problems with openshell systems. Restricted and unrestricted HF methods (elementary idea).discussion of electron correlation.

Reference Books:

1. Atkins P. W., Physical Chemistry, Oxford University Press, New York.
2. Levine I. N., Physical Chemistry, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
3. Adamson A. W., Physical Chemistry of Surfaces, John Wiley and Sons. Other References 1. Day M. C. and Selbin J., Theoretical Inorganic Chemistry. 2. Pashley R. M. and Karaman M. E., Applied Colloid and Surface

<u>Surface Chemistry</u>

Unit 1 Surface Chemistry

Adsorption Surface tension, capillary actions, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces.

Unit 2 Surface Chemistry in Solid Liquid System

The Solid-Liquid Interface Surface energy from solubility changes, surface energy from immersion, contact angle, contact angle hysteresis, experimental methods and measurement of contact angle, theories of contact angle phenomena, adsorption of non-electrolytes from dilute solutions, irreversible adsorption, adsorption in binary liquid systems, adsorption of electrolytes.

Unit 3 Surface Characterization Techniques

Ultra-high vacuum for surface studies, Low energy electron diffraction, Photoelectron spectroscopy, Inverse photoemission spectroscopy, Scanning probe microscopy, Auger electron spectroscopy, Infrared spectroscopy, High resolution electron.

Unit 4 Surface Chemistry and Micelles

A Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation. Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm.

Micelles-Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, micro emulsions, reverse micelles

Reference Books

1. Somorjai, G.A.; Introduction to surface chemistry and catalysis, 2nd edition; 2010; WileyBlackwell.

2. Singh N. B., Gajbhiye N. S. and Das S. S. Comprehensive Physical Chemistry, New Age publishers, New Delhi.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Semester - III

Course Name: Industrial Chemistry Laboratory -1	**Course Code: MSIC-305P**
Credit 4	**Practical course -5**

Course Objectives

The main objective of this course is to :

1. Understand agrochemical chemistry – Identify and analyze fertilizers, pesticides, and other agriculturally important chemicals.
2. Explore textile chemistry – Study the properties, identification, and chemical treatment of natural and synthetic fibers.
3. Learn polymer chemistry – Synthesize and characterize basic polymers, thermoplastics, and thermosetting materials.
4. Develop practical skills – Gain proficiency in laboratory techniques including titrations, spectroscopy, microscopy, extraction, and colorimetric tests.
5. Apply safety and environmental practices – Handle chemicals responsibly and dispose of laboratory wastes safely.

Course Outcomes

CO1: Detect and analyze agrochemicals – Test for nitrates, phosphates, and other active ingredients in fertilizers and pesticides.

CO2: Synthesize and study agrochemical products – Prepare urea-formaldehyde fertilizer or other simple agrochemicals.

CO3: Identify textile fibers – Distinguish between natural and synthetic fibers using chemical and microscopic methods.

CO4: Test textile properties – Examine fiber solubility, dye absorption, and presence of finishing agents such as starch.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

CO5: Prepare and characterize polymers – Synthesize PVA films, phenol-formaldehyde resin, and study their physical properties.

CO6: Apply lab safety and environmental responsibility – Demonstrate proper chemical handling, storage, and disposal techniques.

Course Description

This laboratory course provides practical exposure to the chemistry and applications of agrochemicals, textile materials, and polymers. The course emphasizes experimental techniques, observation, data analysis, and interpretation, reinforcing theoretical knowledge from related chemistry courses. It also introduces students to safe laboratory practices, chemical handling, and environmental considerations in industrial chemistry.

Outlined Syllabus

1. To determine the presence of nitrate ions in fertilizers.
2. Preparation of Simple Urea Formaldehyde Fertilizer.
3. To detect the presence of organophosphorus in pesticides.
4. To identify natural and synthetic fibers.
5. Detect starch used in textile finishing.
6. To study the affinity of natural and synthetic dyes for different fibers.
7. To prepare a simple polymer film.
8. To prepare a Phenol-Formaldehyde Resin
9. To compare properties of natural and synthetic polymers.

Reference Books:

1. Plimmer, Jack R. — Encyclopedia of Agrochemicals, 1st edition, 2003, Wiley-VCH.
Wiley-VCH
2. Cutler, Horace G. & Cutler, Stephen J. (eds.) — Biologically Active Natural Products: Agrochemicals, 1st edition, 1999, CRC Press
3. Michalis K. Konsolakis (ed.) — Surface Chemistry and Catalysis, 1st edition, 2016, MDPI Books.
4. Saunders, K. J. — Organic Polymer Chemistry: An Introduction to the Organic Chemistry of Adhesives, Fibres, Paints, Plastics and Rubbers, 2nd edition, 1988, Springer.
5. Koltzenburg, Sebastian; Maskos, Michael; Nuyken, Oskar — Polymer Chemistry, 1st edition, 2017, Springer.

Semester - III

Course Name: Industrial Chemistry Laboratory -2	**Course Code: MSIC-306P**
Credit 4	**Practical course - 6**

Course Objectives

1. Identify and characterize common industrial minerals based on physical and chemical properties.
2. Apply gravimetric and titrimetric methods for quantitative estimation of mineral components such as silica, alumina, lime, and iron oxides.
3. Determine volatile content and loss on ignition for various minerals.
4. Perform qualitative analysis of mineral cations using flame and precipitation tests.
5. Understand and demonstrate laboratory preparation techniques for industrial mineral products such as plaster of Paris and hydrated lime.
6. Develop skills in accurate observation, recording, and analysis of experimental data.

Course Outcomes

Student will be able to

CO1: Identify industrial minerals and distinguish them using physical and chemical tests.

CO2: Estimate quantitatively the content of major oxides like SiO_2, Al_2O_3, CaO, and Fe_2O_3 in mineral samples.

CO3: Calculate loss on ignition (LOI) and evaluate the volatile content of minerals.

CO4: Perform flame and precipitation tests to identify metallic ions in minerals.

CO5: Prepare small-scale industrial products (e.g., plaster of Paris, soda ash, hydrated lime) and understand their laboratory synthesis.

CO6: Apply laboratory techniques to ensure accuracy, reproducibility, and safe handling of chemicals and minerals.

Course Description

This laboratory course is designed to provide hands-on experience in the analysis, identification, and characterization of industrial minerals. Students will learn to determine the chemical composition, physical properties, and industrial relevance of various minerals such as limestone, bauxite, gypsum, clay, and iron ore.

The course emphasizes gravimetric, titrimetric, and qualitative analytical techniques, along with simple preparation of mineral-based products. Safety, accuracy, and systematic observation are integral to all experiments.

Outline Syllabus

1.To identify physical and chemical properties of common industrial minerals.
2. Gravimetric Analysis of Minerals
3. To determine moisture, carbonates, or other volatile components in given mineral.
4.Determination of carbonate content in limestone by acid-base titration.
5.Determination of total hardness in water using EDTA (optional, related to industrial minerals).
6. Flame test for Na^+, K^+, Ca^{2+}, Ba^{2+} in mineral salts.
7. Precipitation reactions to confirm Ca^{2+}, Mg^{2+}, Al^{3+}.
8. Preparation of plaster of Paris from gypsum.
9. Preparation of soda ash from sodium carbonate (small scale).
10.Preparation of hydrated lime from quicklime.
11. Determination of specific gravity of minerals using a pycnometer.
12. Estimation of iron oxide (Fe_2O_3) in iron ore using simple gravimetric method.

Reference Books:

1. “Physicochemical Methods of Mineral Analysis” — Alastair W. Nicol (Ed.)
2. “Applied Mineralogy: Applications in Industry and Environment” — Swapna Mukherjee
3. “Elements and Mineral Resources” — Joaquim Sanz, Oriol Tomasa, Abigail Jimenez-Franco, Nor Sidki-Rius
4. “Techniques for Analysis of Mineral Raw Materials” — Carlos Pérez Bergmann
5. “Analytical Chemistry in the Exploration, Mining and Processing of Materials” — A. Strasheim, T. W. Steele (Eds.)
6. “Ullmann’s Encyclopedia of Industrial Chemistry” — Fritz Ullmann (Ed.)
7. “Mineral Scales in Biological and Industrial Systems” — Zahid Amjad (Ed.

Semester IV

Course Name: Pharmaceutical Chemistry	Course Code: MSIC-401
Credit 4	Core Course -11

Course Objective

1. To explain receptor theory, drug-receptor interactions, binding forces, and structure-activity relationships (SAR).
2. To describe the chemistry of drug absorption, distribution, metabolism, and excretion (ADME).
3. To introduce and apply Computer-Aided Drug Design (CADD), including QSAR, molecular modeling, and docking studies.
4. To understand the synthesis and reactivity of heterocyclic compounds and prepare drugs from various therapeutic classes.
5. To utilize modern analytical techniques such as UV-Vis, IR, NMR, Mass Spectrometry, HPLC, and GC for drug characterization and quantification.
6. To apply principles of GMP, validation, stability testing, and impurity profiling in drug development and manufacturing.

Course Outcomes

CO1: Demonstrate knowledge of drug-receptor interactions and predict pharmacological activity using SAR.

CO2: Evaluate the pharmacokinetic properties of drugs and understand their impact on efficacy and safety.

CO3: Apply computational tools like QSAR and molecular docking to assist in rational drug design.

CO4: Execute the synthesis of heterocyclic compounds and therapeutic agents with a clear understanding of reaction mechanisms.

CO5: Perform accurate drug analysis using advanced spectroscopic and chromatographic techniques.

CO6: Implement quality assurance and control protocols in line with GMP standards.

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Course Description

This course provides an in-depth understanding of the principles and applications of medicinal chemistry, drug design, synthesis, and pharmaceutical analysis. It covers the fundamentals of drug-receptor interactions, structure-activity relationships (SAR), and pharmacokinetics (ADME), along with modern computational approaches like QSAR, molecular modeling, and docking studies. Students will explore the synthesis of key therapeutic agents, focusing on heterocyclic compounds and clinically important drugs. The course integrates theoretical knowledge with practical applications in drug discovery, development, and quality evaluation, including natural product-based pharmaceuticals.

Outlined Syllabus

Unit 1 Medicinal Chemistry and Drug Design

Drug Action Fundamentals: Concepts of receptor theory, drug-receptor interaction, binding forces, and structure-Activity Relationships (SAR).

Pharmacokinetics (ADME): Chemistry of Absorption, Distribution, Metabolism (biotransformation), and Excretion of drugs.

Computer-Aided Drug Design (CADD): Introduction to QSAR (Quantitative Structure-Activity Relationships), molecular modeling, and docking studies.

Unit 2 Synthesis of Drugs

Heterocyclic Chemistry: Focus on the synthesis and reactivity of key heterocyclic rings present in pharmaceuticals (e.g., pyridine, pyrimidine, indole).

Targeted Synthesis: Detailed synthesis and reaction mechanisms for various therapeutic classes like analgesics (e.g., Paracetamol), antibiotics (e.g., Penicillins), cardiovascular drugs, and anti-infectives.
Pharmaceutical Analysis and Quality Control
Modern Analytical Techniques: Application of Spectroscopy (UV-Vis, IR, NMR, Mass Spectrometry) and Chromatography (HPLC, GC) for drug characterization and quantification.

Unit 3 Quality Assurance (QA) & Control (QC)

Concepts of Good Manufacturing Practices (GMP), validation, stability testing, and impurity profiling in the pharmaceutical industry.

Natural Products: Extraction, purification, and structural elucidation of active pharmaceutical ingredients (APIs) from natural sources (phytochemicals).

Reference Books

1. Medicinal Chemistry, Ashutosh Kar, New Age International.
2. Textbook of Drug Design and Discovery, Kristian Stromgaard, Christoffer A. Olsen, Jan M. Krieg, CRC Press.
3. Foye’s Principles of Medicinal Chemistry, Thomas L. Lemke, David A. Williams, Lippincott Williams & Wilkins.
4. Computer-Aided Drug Design: Methods and Applications, Thomas J. Perun, Humana Press.
5. Heterocyclic Chemistry, J.A. Joule, Keith Mills, Wiley.
6. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Jerry March, Wiley.
7. Pharmaceutical Analysis: A Textbook for Pharmacy Students and Pharmaceutical Chemists, David G. Watson, Churchill Livingstone.
8. Good Manufacturing Practices for Pharmaceuticals, Graham Bunn, CRC Press.

Semester - IV

Course Name: Green Chemistry/ Polymer Chemistry/ Material Chemistry/Computational Chemistry	**Course Code: MSIC-402A/ MSIC-402B/ MSIC-402C/ MSIC-402D**
Credit 4	**Discipline Elective Course - 4**

Course Objectives

With the environmental concern and shrinking resources acquiring enormous proportions, it has become imperative to devise safer alternative materials and technology that would ensure the human sustenance. This course intends to take the students through the newer, environment friendly products and procedures and incite them to take a more holistic view of different chemical processes.

Course Outcomes

CO1: Explain the field of green chemistry.
CO2: Acquire knowledge of the 12 principles of green chemistry.
CO3: Develop an understanding of cleaner production and green synthesis methods
CO4: Acquire the Knowledge of catalysis, and microwave theory.
CO5: Appreciate the Principle of Photochemical

Green Chemistry

Unit l Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/Obstacles in the pursuit of the goals of Green Chemistry. Definition and concepts: green chemistry; sustainable consumption of resources; individual and community level participation such as small-scale composting pits for biodegradable waste.

Unit 2 Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy).

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road. Meerut

Unit 3 Cleaner Production

The Cleaner Production Concept , Why Cleaner Production , Difference With End of Pipe Concept, Cleaner Production and Sustainable Development, Implementation of Cleaner Production , Change of Raw Material, Technology Change, Good Operating Practice, Product Change, On Site Reuse And Recycling, Who Is Responsible For Cleaner Production, Government Rules, Green Synthesis of Nano Particles.

Unit 4 Green Chemical Strategies for Sustainable Development

Areas of green chemistry, Reaction mass balance-Atom Economy, Evaluation for Chemical Reaction Efficiency, Green Solvents/ reaction Media, Catalysis and Bio catalysis. Microwave oven as a reactor, Theory of Microwave Heating.

Unit 5 Photochemical Degradation

An Eco-friendly Approach of Waste Treatment
Photochemical Principles, Heterogeneous Photo-catalysis, Homogeneous Photo-degradation, photo oxidation, Direct Photo-degradation, Gas phase Detoxification, Equipments and applications.

Reference Books

1., P., and Williamson, T. C., Green Chemistry Frontiers in Benign Chemical Synthesis and Processes, Oxford University Press (1999).
2.Ahluwalia, V. K., and Kidwai, M., New Trends in Green Chemistry, Anamaya Publishers (2004).
3.Protective Groups in Organic Synthesis, Peter G. M. Wuts, T.W. Greene.
4.Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).

Polymer Chemistry

Unit 1 Basics Importance of polymers

Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain, ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization n homogenous and heterogeneous systems.

Unit 2 Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testingtensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

Unit 3 Structure and Properties

Morphology and order in crystalline polymers, configurations of polymer chains. Crystal structure of polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties, crystalline melting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg. Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

Unit 4 Polymer Processing

Plastic, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

Reference Books

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.

2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. inaki and R.M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional

Material chemistry

Unit 1 Multiphase Materials

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

Unit 2 Glasses, Ceramics, Composites and Nanomaterials

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced, firbe-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

Unit 3 Thin Films and Langmuir-Blodgett Films

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuiur-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit 4 Liquid Crystals

Mesomorphic ehavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit 5 Polymeric Materials

Molecular shape, structure and configuration, crystallinity, stress-strain ehavior, thermal ehavior, polymer types and their applications, conducting and ferro-electric polymers.

Unit 6 Ionic Conductors

Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Unit 7 High Tc Materials

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials.

Reference Books

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag.
7. Inorganic Materials:Recent Advances,Editors D.Bahadur et al.,Narosa
8. Ion Conducting Materials: Theory and Applications, Editor A. R. Kulkarni, Narosa

Computational chemistry

Unit 1Basic Computer system

Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and
Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/ String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High-Level languages (Machine language, Assembly language; QBASIC, C, C++, FORTRAN 90&95); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application

Unit 2 Introduction to Python

Why Python ? Python coding environment setup, Pythonas an interpreted language, Brief history of Python, Uses of Python (including artificial intelligence and machine learning), Applications of Python in Chemistry

Unit 3Coding in Python

(i) Basic syntax including constants and variables, Operators, Data Types, Declaring and using Numeric data types: int, float, string etc.

(ii) Program Flow Control Conditional blocks: if, else and else if, simple FOR loops, FOR loop using ranges, string, list and dictionaries. Use ofwhile loops, Loop manipulation using pass, continue, break and else.

(iii) Complex data types: String, List,Arrays,TuplesandDictionary,Stringoperationsand manipulationmethods,List operations including slicing, in-built Python Functions.

(iv) Python packages - usage of numpy and scipyfor mathematical computations.

Unit 4 Numerical Methods in Chemistry

Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods and binary bisection) with examples of polynomial equations used in chemistry; Numericaldifferentiation – finite difference method (backward, centraland forward), Numerical integration - Trapezoidal and Simpson’s rule to calculate area under the curves for chemistry problems, e.g., entropy calculations, Simultaneous equations, Statistical analysis- mean,variance, standard deviation, error, Curve fitting – linear regression, Solving Schrödinger’s equation using Python packages.

Reference Books

1. Computer Fundamentals by P.K. Sinha.
2. Fundamentals of Computers by V. Rajaraman.
3. Python Programming: An Introduction to Computer Science by John Zelle.
4. Numerical Methods for Scientists and Engineer by R.W. Hamming.
5. Computational Chemistry Using the PC by Donald W. Rogers

Semester - IV

Course Name: Medicinal Chemistry/ Environmental Chemistry/ Photochemistry/ Supramolecular Chemistry	**Course Code: MSIC-403A/ MSIC-403B/ MSIC-403C/ MSIC-403D**
Credit 4	**Discipline Elective Course - 4**

Medicinal Chemistry

Unit 1 Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR) factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations.

Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR.

Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constant, steric, Shelton and surface activity parameters and redox potentials.

Unit 2 Pharmacokinetics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Unit 3 Pharmacodynamics

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotic, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit 4 Antineoplastic

Agents Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine,

K V Subharti College of Science
S V Subharti University
NH-58 Byepass Road, Meerut

cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Unit 5 Antibiotics

Cell wall biosynthesis inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Reference Books

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's: Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I, Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

Environmental Chemistry

Unit 1 Environment

Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Bio distribution of elements.

Unit 2 Hydrosphere

Aquatic pollution- inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand. Purification and treatment of water.

Unit 3 Soils

Composition, micro and macro nutrients, Pollution of fertilizers, pesticides and metals. Unit IV Atmosphere Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals chlorofluorohydrocarbons. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Unit 4 Industrial Pollution

Pollution from cement, sugar, distillery, drug; paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs etc.

Unit 5 Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Reference Books

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.

5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman.

<u>Photochemistry</u>

Unit 1 Basics of photochemistry

Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative process, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

Unit 2 Properties of Excited States

Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Biomolecular deactivation-quenching.

Unit 3 Excited States of Metal Complexes

Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes. Charge-transfer spectra, charge transfer excitations, methods for obtaining chargetransfer spectra.

Unit 4 Photosubstitution

Photo oxidation and photo reduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Unit 5 Redox Reactions by Excited Metal Complexes

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium2+, (bipyridyl complex, comparison with Fe (bipy)3); role of spin-orbit coupling, life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high-energy products, chemical energy into light.

Unit 6 Metal Complex Sensitizers

Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Reference Books:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
4. Co-ordination Chem. Revs., 1975, 15, 321; 1981, vol. 39, 121, 131; 1990, 97, 313.
5. Photochemistry of Co-ordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
7. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
8. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
9. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
10. Introductory Photochemistry, A. Cox

Supramolecular Chemistry

Unit 1 Fundamentals of Supramolecular Chemistry

Terminology and definitions in supramolecular chemistry. Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; cation-pi, anionpi, pi-pi interactions and Van der Waal forces. Solvent and solution properties, solvation and hydrophobic effect. Binding constants; definition and use, determination of binding constant by physical methods.

Unit 2 Molecular Recognition

Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Structure and function of receptors with molecular clefts, Synthesis and applications of supramolecular host with multiple hydrogen bonding sites (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine, ionophores) as cation and anion binding receptors and receptors for ionpair recognition.

Unit 3 Reactivity and Catalysis

Organocatalysis mediated through hydrogen bonding, preconcentration, self-assembly of catalysts and preorganisation of catalyst-substrate systems. Influence of organization (effective molarity) on catalysis, Catalytic acyl transfer, acid-base catalysis, catalysis hydrolysis as ATPase mimic.

Unit 4 Applications of Supramolecular Materials

Basic principles and applications, Covalent organic frameworks, Metal organic frameworks, Host-guest complexation, micelles, polymers, Multifunctional catalysis.

Reference Books

1. Supramolecular Chemistry: from Molecules to Nanomaterials Eds. by P.A. Gale and J.W. Steed (2012).
2. Modern Supramolecular Chemistry by F. Diederich, P. J. Stang, R. T. Tykwinski (2008). .
3. Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner, K. J. Wallace (2007).
4. Supramolecular Chemistry by J.W. Steed and J.L. Atwood (2011).
5. Supramolecular Chemistry: Concepts and Perspectives by J.-M. Lehn, Wiley VCH, Weinheim (1995).