ST JOSEPH'S UNIVERSITY

BENGALURU - 27

SCHOOL OF CHEMICAL SCIENCES

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ANALYTICAL CHEMISTRY

2024-2027

A Public-Private-Partnership University under RUSA 2.0 of MHRD (Government of India), established by the Karnataka Govt. Act No. 24 of 2021.

FROM 2024 ONWARDS

Department of Chemistry

The Postgraduate programme in chemistry is designed to give students a good foundation in Chemistry and develop their problem-solving and experimental skills so that they are well prepared for further studies in specialized areas of Chemistry or for employment in academic institutions and industry.

Mission statement:

- To promote among our learners the skills of thinking, experimentation and application of the knowledge gained.
- To promote concern for the environment and to develop an appreciation for green chemistry.
- To prepare our students for life in the larger community.

Benchmark Statements for the Course:

- To instill in students a sense of enthusiasm for chemistry, an appreciation of its application in different contexts, and to involve them in intellectually stimulating and satisfying experiences of learning and studying.
- To provide students with a broad and balanced foundation of chemical knowledge and practical skills.

Teaching-Learning:

Although the lecture method is extensively used, the students are also encouraged to do self-study through other activities like assignments, seminars, quizzes, viva voce etc.

Co-curricular Activities:

The Chemical Society for P.G. students provides them with a platform to interact with students from other institutions and also with eminent scientists from universities, other academic institutions and industries.

Course Details: The course details for the P.G. programme are as follows:

SUMMARY OF CREDITS

SEMESTER	PAPER CODE AND TITLE	NO. OF TEACHING HOURS/week	NO. OF CREDITS	TOTAL MARKS
SEMESTER I				
THEORY				
Paper I	CH7124: Inorganic Chemistry - I	4	04	100
Paper II	CH7224: Organic Chemistry - I	4	04	100
Paper III	CH7324: Physical Chemistry - I	3	03	100
Paper IV	CH7424: Spectroscopy -I	4	04	100
Paper V	CH7524: Principles of Chemical Analysis	4	04	100
PRACTICAL				
Paper I	CH7P1 Inorganic Chemistry Practical I	4	1.5	50
Paper II	CH7P2 Inorganic Chemistry Practical II	4	1.5	50
Paper III	CH7P3 Organic Chemistry Practical I	4	1.5	50
Paper IV	CH7P4 Organic Chemistry Practical II	4	1.5	50
		TOTAL	25	500
SEMESTER II				
THEORY				
Paper I	CH8124: Inorganic Chemistry II	4	04	100
Paper II	CH8224: Organic Chemistry II	4	04	100
Paper III	CH8324: Physical Chemistry II	4	04	100
Paper IV	CH8424: Spectroscopy II	4	04	100
Paper V	CH8524: Separation Techniques	3	03	100

PRACTICAL				
Paper I	CH8P1 Physical Chemistry Practical I	4	1.5	50
Paper II	CH8P2 Physical Chemistry Practical II	4	1.5	50
Paper III	CH8P3 Preparation and characterization - I	4	1.5	50
Paper IV	CH8P4 Preparation and characterization - II	4	1.5	50
		TOTAL	25	600

SEMESTER	PAPER CODE AND TITLE	NO. OF TEACHING HOURS	NO. OF CREDIT S	TOTAL MARKS
SEMESTER III				
THEORY				
Paper I	CH9125: Biological Chemistry	4	4	60
Paper II	CH9225: Organometallic Chemistry	4	4	60
Paper III	CH9325: Electrochemistry and Electroanalytical Techniques	3	3	45
Paper IV	CH9425 Solid State Chemistry	4	4	60
Note: Students can choose one of the departmental elective from Paper V-A or V-B				
PRACTICAL				
Paper I	CH9P1: Applied Analysis-I	4	1.5	50

Paper II	CH9P2: Applied Analysis-II	4	1.5	50
Paper III	CH9P3: Advanced Methods of Analysis –I	4	1.5	50
Paper IV	CH9P4: Advanced Methods of Analysis –II	4	1.5	50
		TOTAL	**6**	**200**
SEMESTER IV				
Paper I	CH0125: Applied Analysis	4	4	60
Paper II	Dept Electives CHDE 0225: Chemistry of Materials CHDE 0325: Green Chemistry and Diversity of its Applications CHDE 0425: Forensic Chemistry CHDE 0525: Supramolecular Chemistry	4	4	60
	CH0PR PROJECT WORK	**42/week**	**14**	**100**
	IGNITORS/ OUTREACH		**04**	
Total No. of Credits: 26				
KEY WORDS: DE – Departmental Elective and OE – Open Elective				

Note: One credit is equivalent to one hour of teaching (lecture or tutorial) or three hours of practical work/field work per week.

CREDITS FOR M.Sc. CHEMISTRY						
I -II SEMESTER						
	T/P	**Number Of Teaching Hours Per Week**	**CREDITS**	**Total Teaching Hours per Semester**	**TOTAL CREDITS IN ONE SEMESTER**	**TOTAL CREDITS IN ALL SEMESTERS**
Optional Subjects					25	25 x 2 = 50
A	T	4	4	60		
B	T	4	4	60		
C	T	4	4	60		
D	T	4	4	60		
E	T	3	3	45		
Practical-I	P	4.5	1.5	50		
Practical –II	P	4.5	1.5	50		
Practical-III	P	4.5	1.5	50		
Practical –IV	P	4.5	1.5	50		
III SEMESTER						
Optional Subjects					23	23
A	T	4	4	60		
B	T	4	4	60		
C	T	3	3	45		
D	T	4	4	60		
Practical-I	P	4.5	1.5	50		
Practical –II	P	4.5	1.5	50		
Practical-III	P	4.5	1.5	50		
Practical –IV	P	4.5	1.5	50		
Outreach Programme			2			
IV SEMESTER						
A	T	4	4	60	25	25
Dept. elective	T	4	4	60		
PROJECT	P	42	15	100		
IGNITORS			2			
TOTAL						**98**

FIRST SEMESTER
THEORY PAPERS

Semester	I
Paper code	CH 7124
Paper title	INORGANIC CHEMISTRY – I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. CHEMICAL BONDING **(10+2) hours**

(Lewis Structures: The octet rule, resonance, VSEPR theory). Valence Bond theory: homonuclear diatomic molecules (H_2& N_2), polyatomic molecules (H_2O), hypervalence (PCl_5 and SF_6), hybridization. Molecular orbital theory: introduction to wave functions for molecular orbitals, ***LCAO approach***, symmetry and overlap, symmetry of molecular orbitals, ***homonuclear diatomic molecules(H_2 to O_2)*** and molecular ions, heteronuclear diatomic molecules (HF, CO, BeH_2 and ICl), bond order and magnetic property. Polyatomic molecules – molecular orbitals of NH_3, hypervalence in the context of molecular orbitals (SF_6), molecular shapes in terms of molecular orbitals - Walsh diagram (for XH_2 molecules), calculation of bond enthalpy, Ketelaar triangle, Bent's rule, quadruple and agostic bonds with examples.

2. THE STRUCTURES OF SIMPLE SOLIDS **(16+2) hours**

Unit cells and the description of crystal structures - the close packing of spheres, holes in close-packed structures. Structures of metals and alloys, polytypism, nonclose-packed structures, polymorphism of metals, atomic radii of metals, Goldschmidt correction. Alloys - substitutional solid solutions, interstitial solid solutions of nonmetals, intermetallic compounds, Zintl phases. Ionic solids-characteristic structures of ionic solids, binary phases AX_n: rock-salt, cesium-chloride, sphalerite, fluorite, anti-fluorite, zinc blende and wurtzite, nickel arsenide and rutile, $CdCl_2$ and CdI_2 layered structures, ternary phases ABX_3, AB_2X_4 and $B(AB)X_4$: perovskite, spinel and inverse spinel structures. Rationalization of structures - ionic radii, radius ratio, structure maps. The energetics of ionic bonding, lattice enthalpy and Born–Haber cycle, calculation of lattice enthalpies, Born-Lande equation-derivation - comparison of experimental and theoretical values - Kapustinskii equation, volume-based thermodynamic approach for calculation of lattice energy, consequences of lattice enthalpies. ***Defects and nonstoichiometry - Intrinsic point***

defects - Schottky defect, Frenkel defect -Predicting defect types - Extrinsic point defects-F-centre, nonstoichiometric compounds.

3. CHEMISTRY OF THE MAIN GROUP ELEMENTS (17 + 3) hours

Polymorphism of carbon, phosphorus and sulphur: Structure-property correlation in diamond and graphite, intercalation compounds of graphite, carbon nanotubes-types and preparation, structure of fullerene(C_{60}). Differences among white phosphorus, black phosphorous and red phosphorous with special emphasis on structural aspects. Cyclosulphur and polycatenasulphur. Boranes: Classification, preparation of higher boranes by Stock's method and pyrolysis of diborane, reactions of diboranes with Lewis bases- symmetric and unsymmetric cleavage, types of bonds in higher boranes- the styx number, formulae for arriving at the number of 2-centre and 3-centre bonds in boranes, Wade's rules as applied to boranes, Geometrical and Lipscomb's semitopological structures of B_4H_{10}, B_5H_9, B_5H_{11}, B_6H_{10} and $B_{10}H_{14}$. Carboranes: classification, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$. Metallocarboranes: preparation and structures. Borazines: Preparation, properties and structure. Difference in chemical properties between borazine and benzene, borazine derivatives (N& B substituted). Structure, preparation and applications of boron nitride. Phosphazenes: Classification, Cyclophosphazenes-$(NPCl_2)_3$ and $(NPCl_2)_4$- preparation and structure, Linear polyphosphazenes- preparation and applications. Sulphur-nitrogen compounds: (S_xN_y: x=y, x≠y). Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates. ***Silicates- Classification and structures of ortho, pyro, chain, cyclic, sheet and three-dimensional silicates***. Silicon-Silicon (sil-ane, -ene, -yne) multiple bonded systems.

4. ACIDS AND BASES (5 + 1) hours

(Review of acid- base concepts– Bronsted, Lewis and solvent system definitions of acids and bases, generalized acid-base concept.) Systematics of Lewis acid-base interactions: Drago - Wayland equation. Factors affecting strength of Lewis and Bronsted acid/base strengths with special emphasis on steric effects and solvation effects. ***HSAB concept- Pearson's principle***, ***classification of acids and bases as hard and soft***, Bronsted acid-base strength versus hardness and softness, symbiosis, theoretical basis of hardness and softness. Frustrated Lewis pair: Use in small molecule (H_2) activation.

5. NONAQUEOUS SOLVENTS 4 hours

Chemistry in non-aqueous media – Classification of solvents, levelling effect, acid-base reactions in BrF_3, N_2O_4 and molten salts. Reactions in super critical fluids. Ionic liquids-preparation of 1-butyl-3-methylimidazolium hexafluorophosphate, properties and applications of ionic liquids.

REFERENCES

1. Inorganic Chemistry, 7th Edn., M. Weller, J. Rourke, T. Overton, F. Armstrong, Oxford University Press, 2018.
2. Inorganic Chemistry, 5th Edn., C. E. Housecroft, A. G. Sharpe, Pearson Education Ltd., 2018.
3. Principles of Inorganic Chemistry, 2nd Edn., John Wiley and Sons, 2022.
4. Foundations of Inorganic Chemistry, G. Wulfsberg, University Science Books 2018.
5. Fundamental Concepts of Inorganic Chemistry, Volume 1, 3rd Edn., A. K. Das, CBS Publishers & Distributers Pvt. Ltd., 2020.
6. Supercritical Fluids as Solvents and Reaction Media- G. Brunner, Elsevier, 2004.
7. Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edn., J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Pearson Education Asia Pvt. Ltd., 2006.
8. Basic Inorganic Chemistry, 3rd Edn., F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and Sons, 1995.
9. Concise Inorganic Chemistry, 5th Edn., J. D. Lee, Blackwell Science Ltd., 1996.
10. Chemistry of Elements, 2nd Edn., N. N. Greenwood and A. E. Earnshaw, Reed Educational and Professional Publishing Ltd., 1997.
11. Chemistry of non-Metals, R. Stuedel, D. Scheschkewitch, Walter de Gruyter GmbH, 2020.
12. Inorganic Chemistry, 5th Edn., G. L. Miessler, P. J. Fischer, D. A. Tarr, Pearson Education Inc., 2014.

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

LO1	Knowledge	Recall concepts, laws, relationships, molecular structures in chemical bonding, crystal structures in solid state, valence bond and molecular orbital theories for diatomic and polyatomic molecules, Bent's rule, quadruple and agostic bonds, main group elements, uses of P–N, P–S and S–N compounds acids and bases, non-aqueous solvents List the properties of ionic liquids and molten salts. Identify the type of bonding from Ketelaar triangle, delta and agostic bonds Define unit cell, polytypism, polymorphism, lattice energy Draw the overlapping of atomic orbitals, hybrid and molecular orbitals, close packing of spheres, holes in close-packed structure
LO2	Understand	Explain hypervalence using hybridisation, magnetic

		properties using MOT, Structures of metals and alloys, the linear combination of atomic orbitals, overlapping to form the molecular orbitals, bonding in boranes, borazines and phosphazenes; the properties of non-aqueous solvents, different acid-base theories, structures of crystalline solids. Classify acids and bases as hard and soft, the type of compound based on Ketelaar triangle Describe syntheses of compounds of main group elements and LCAO approach. Discuss the chemistry of B, N, P, S-based compounds, factors affecting acid-base strength
LO3	Apply	Predict molecular structure based on valence bond and molecular orbital theory, the structures adopted by simple ionic solids, magnetic properties from MOT, structure using Bent's rule, defect types - Extrinsic point defects-F-centre, nonstoichiometric compounds. Formulate styx numbers of closo, nido, arachno polyhedral structures. Calculate the bond order of diatomic molecules/ions using MOT, bond enthalpy, density of a solid, metallic radii, lattice energy using Born–Haber cycle, Born-Lande equation, Kapustinskii equation, volume-based thermodynamic approach for calculation of lattice energy, the number of skeletal electron pairs using Wade's rule.
LO4	Analyze	Compare and contrast the linear and bent molecules using Walsh diagram, experimental and theoretical lattice energy values, number of B-B-B, B-H-B 3c-2e bonds of boranes, carboranes, metallocarboranes.
LO5	Evaluate	Compare the structure-property correlation in allotropes of C, S and P Interpret the photoelectron spectrum to correlate the MO energies for a compound. Deduce the structure of carborane from given higher borane Assess the type of acid-base nature of given compound
LO6	Create	Construct LCAO for complex molecules Predict the formula of boranes from the data given Propose the STYX number of a given borane.

Semester	I
Paper code	CH 7224
Paper title	ORGANIC CHEMISTRY – I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. STRUCTURE, REACTIVITY & REACTION MECHANISMS (11+4) hours

<u>Resonance, field effects, hyperconjugation, steric effects and steric inhibition of resonance on reactivity</u>.

Quantitative treatment of field and resonance effects – Hammett and Taft equations.

Basic concepts of reaction mechanisms; thermodynamics and kinetics of reactions, Thermodynamic vs. kinetic control, Hammond postulate, microscopic reversibility, Curtin – Hammett principle.

Reactive intermediates: Generation, structure, stability and reactivity of (*carbocations, carbanions, carbon free radicals,)* carbenes and nitrenes.

Methods of determining mechanisms: Characterization of intermediates, kinetics, stereochemistry, kinetic isotopic effects, isotopic labeling experiments and solvent effects.

2. STEREOCHEMISTRY (15+2) hours

Molecules with 2 and 3 stereocenters – Interconversion of perspective, Fischer, sawhorse and Newman structures. R-S notation of molecules with more than 2 chiral centers, erythro/threo nomenclature, meso compounds, systems with pseudoasymmetriccentres.

Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes, P, M notations. Helicity – helicenes, end substituted benzphenanthrenes. ***<u>Classification of racemic modifications, E-Z configuration notation. In-out isomerism</u>***.

Homotopic, enantiotopic and diastereotopic atoms, groups and faces; prochirality; *pro-R/S, Re/Si* configuration notations.

Conformations of mono and di-substituted ethanes. (*Energy profiles of conformations of ethane, propane, butane and cyclohexane).* ***<u>Conformations of mono-substituted cyclohexanes</u>***, conformation and configurational details of di-substituted cyclohexanes.

Fused rings and bridged rings, nomenclature of bridged systems, decalins, norbornanes, bicyclo [2.2.2] octane.

3. ALIPHATIC NUCLEOPHILIC SUBSTITUTION **11 hours**

Substitution at sp^3 carbon atom; limiting cases- S_N1 and S_N2 mechanisms. Factors influencing S_N1 and S_N2 reactions – substrate, leaving group, nucleophile and solvent. Ambident substrates and nucleophiles – regioselectivity. Borderline cases: intermediate mechanism. Neighboring group participation, non-classical carbocations. S_Ni mechanism. Allylic rearrangements.

Substitution at a trigonal carbon atom – the tetrahedral mechanism, formation of acid derivatives, cleavage of esters and N-acylation reactions. Substitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

4. ELIMINATION REACTIONS **6 hours**

The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions. Factors influencing E1, E1cB and E2 reactions – substrate, leaving group, nucleophile and solvent. Substitution vs. elimination. Pyrolytic eliminations: Hofmann elimination, elimination in esters, xanthates and N–oxides - mechanisms and orientation.

5. AROMATIC SUBSTITUTION **(9+2) hours**

Resonance and molecular orbital interpretation of aromaticity of benzene. Hückel's rule-aromaticity and anti-aromaticity. Aromaticity/anti-aromaticity of benzenoid and non-benzenoid systems and ions.

Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity, ortho/para ratio, ipso attack. Orientation in third substitution. Orientation and reactivity of other ring systems - polycylic aromatic hydrocarbons (naphthalene, anthracene, phenanthrene), heterocyclic systems (pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, and indole). ***Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction***.

Nucleophilic substitution: (S_NAr), S_N1, benzyne and SR_N1 mechanisms.

Reactivity in arenes – effect of substrate structure, leaving group and nucleophile. Reactivity of heterocyclic systems (pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, and indole). von Richter and Smiles rearrangements.

REFERENCES

1. Organic Chemistry, Clayden, Greeves, Warren and Wothers, 2ndEdn, Oxford university press, 2012.
2. March's advanced organic chemistry: Reactions, Mechanisms, and Structure, M. B. Smith, 7th Edn, John Wiley& Sons Inc., 2016.
3. Guidebook to Mechanism in Organic Chemistry (6thEdn), P. Sykes, Pearson education limited, 1986.

4.Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley, 1994.
5. Stereochemistry of organic compounds, D. Nasipuri, Wiley Eastern, New Delhi, 1991.
6. Advanced organic chemistry, Part A, F. A. Carey and J. Sundberg, 5th Edn.,Springer, 2007.
7. Organic chemistry, Volumes I and II, I. L. Finar, Longman, 1999.

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

LO1	Knowledge	Recall principles/concepts in organic reaction mechanisms, stereochemistry, and aromaticity Write general mechanisms of aromatic/aliphatic nucleophilic/electrophilic substitution or elimination reactions List types of reactive intermediates and their methods of generation
LO2	Understand	Explain structure-reactivity relationships based on Hammett equation/Taft equation, chirality, configurational and conformational isomerism, mechanistic details of electrophilic/ nucleophilic substitution, and elimination reactions in aliphatic/ aromatic systems Classify aromatic/antiaromatic/nonaromatic species based on Huckel's rule
LO3	Apply	Predict reactivity/stabilities of reactive intermediates based on structure, stereochemical relationships between molecules, aromaticity in benzenoid and non-benzenoid systems, major products in nucleophilic/electrophilic substitutions, and elimination reactions. Identify prochiral ligands and faces Assign relevant stereochemical notations to prochiral ligands/ faces/stereocentres
LO4	Analyze	Compare and contrast structure-reactivity relationships, andmechanisms of substitution and elimination reactions
LO5	Evaluate	Deduce plausible mechanisms of electrophilic/ nucleophilic substitution and elimination reactions in aliphatic/aromatic systems.
LO6	Create	Design synthesis of any given aliphatic/aromatic compound based on electrophilic/nucleophilic substitution, and elimination reactions.

Semester	I
Paper code	CH 7324
Paper title	PHYSICAL CHEMISTRY – I (Quantum Chemistry)
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. QUANTUM MECHANICS FORMALISM 9hours

(Emergence of quantum mechanics: black body radiation, photoelectric effect and Bohr's model of H-atom).

Matter–wave duality, de Broglie equation; Heisenberg's uncertainty principle; time–independent Schrödinger equation from the equation of a standing wave; physical meaning of wave function, well-behaved wave functions; normalization and orthogonality of wavefunctions.

Operators and operator algebra; eigen value equations, eigen functions and eigen values; hermitian operators and their properties; postulates of quantum mechanics; time–dependent Schrödinger equation.

2. QUANTUM MECHANICAL TREATMENT OF SIMPLE SYSTEMS 12hours

Quantum mechanical treatment of a free particle and a particle in a 1D/3D potential well; eigen values and normalized eigen functions, nodes, symmetry and antisymmetry of eigen functions; quantum mechanical degeneracy (cubic well); accidental degeneracy (tetragonal and orthorhombic wells); application of particle in a 1D potential well model to conjugated systems; quantum mechanical tunneling (no derivation) and examples.

Quantum mechanical treatment of harmonic oscillator, eigen values and normalized eigen functions, zero point energy.

Quantum mechanical treatment of a particle on a ring and rigid rotator; eigen functions and eigen values; quantization of angular momentum.

Quantum mechanical treatment of hydrogen atom; eigen values and orbital functions; expressions of orbital functions in atomic units; radial and angular plots.

3. APPROXIMATE METHODS AND MULTIELECTRON ATOMS 7hrs

Variation theorem and its proof; application to the ground state of helium atom.
Perturbation theory (time-independent); application of perturbation method to the ground state of helium atom (first order correction only).
Multielectron atoms – symmetric and antisymmetric wave functions; ground and excited states of helium; spin orbitals and Pauli principle; Slater determinants; Slater orbitals; effective nuclear charge based on Slater's rules.

4.THEORY OF ANGULAR MOMENTUM 4 hours

Commutation relationships among angular momentum operators; quantum mechanical definition of angular momentum;
Orbital and spin angular momenta; spin-orbit interaction; Clebsch-Gordan series; term Symbols, L-S coupling (Russel–Saunders Coupling), and j-j coupling; Hund's rule of maximum stability.

5. CHEMICAL BONDING 13 hrs

Diatomic molecules: Born-Oppenheimer approximation.
MO theory: LCAO–MO approximation; hydrogen molecule ion (H_2^+); hydrogen molecule; limitations of MO treatment; excited states of H_2 – singlet and triplet states.
Valence bond theory: hydrogen molecule ion (H_2^+); hydrogen molecule (Heitler–London theory).
Hückel MO treatment for simple π–systems-ethyelene, propenyl, cyclopropenyl, butadiene, ***cyclobutadiene and benzene systems. Introduction to extended Hückel calculations.***

REFERENCES

1. Quantum Chemistry, R. K. Prasad, revised edition, New Age International (P) Ltd., 2006.
2. Quantum Chemistry, D. A. McQuarrie, Viva Books Pvt Ltd., 2003.
3. Quantum Chemistry, I. N. Levine, Prentice Hall, India, 2001.

Learning Outcomes: After learning this paper, students should be able to:

LO1	Knowledge	Recall the basic principles of quantum mechanics (QM), such as wave-particle duality and the Heisenberg uncertainty principle, quantization and matter waves. Define the fundamental QM operators such as position, momentum, and energy operators.
LO2	Understand	Explain the postulates, laws and relationships in QM, probability densities, eigen values, Schrödinger equation (SE), normalization and orthogonalization of wave functions, principle of chemical bonding, valence bond and molecular orbital theories. Describe the approximation methods used in QM, the assumptions of Huckel molecular orbital (HMO) theory. Understand how electrons interact within atoms and molecules.

		Summarize the electronic structure of atoms and molecules based on QM principles.
LO3	Apply	Setup and solve Schrödinger equation for simple systems, plot energy levels, problems involving quantum mechanical operators and their eigenstates. Calculate the energy of complex systems using approximation methods Predict the orbital functions and angular momenta of QM systems. Determine the microstates or terms of atomic orbitals. Apply the principles of QM to calculate energy levels, wave functions, and expectation values for simple systems. Use of QM concepts to predict the bond lengths and strengths. Derive HMO for simple conjugated systems.
LO4	Analyse	Differentiate between various QM models and their applications in chemistry, such as the particle in a box model and the harmonic oscillator model. Compare and contrast QM solutions for systems with the corresponding classical mechanical solutions, approximation methods and theories of bonding. Correlate the atomic terms to elucidate spectroscopic data.
LO5	Evaluate	Assess the validity of a QM model/method for a given system, the accuracy of QM calculations by comparing theoretical results such as energy, ionisation potential, dissociation energy with experimental data. Justify the need for rules such as $n+l$ rule, exclusion principle and Hund's rule. Evaluate the strengths and limitations of valence bond theory to predict the ionisation, chemical bonding and resonance structures of systems.
LO6	Create	Construct and solve Schrodinger equation for any given (hitherto unknown) system. Construct determinantal form of wave functions for any conjugated system. Build the molecular orbitals of any π-system by HMO method.

Semester	I
Paper code	CH 7424
Paper title	SPECTROSCOPY – I
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.

2. Text within parenthesis and italics correspond to recall/review.

1. GROUP THEORY IN CHEMISTRY **17+1 hours**

Symmetry elements: identity, inversion center, proper axis, plane of symmetry and improper axis. Equivalent and identical configuration. Symmetry operations and relationship of each symmetry operation with identity. Improper axis of symmetry-operations generated by S_n axis, symmetry conditions for molecular chirality. Definition of groups, properties of group with examples. Subgroups, simple theorems in group theory and group multiplication tables. Conjugate relationships, classes of operations, similarity transformation and order of a group. Symmetries with multiple higher order axis - symmetry operations in tetrahedral and octahedral point groups. Point groups, Schoenflies notations for point groups, ***examples,*** flowchart to determine the point group. Representation of symmetry operations as matrices, reducible and irreducible representations, characters of representations, great orthogonality theorem (without proof) and its corollaries, properties of irreducible representations. Mulliken symbols for irreducible representations. Character tables - C_{nv}, C_{nh}, D_{nh} and C_n point groups (derivation of character table only for C_{2v} and C_{3v} point group). Applications of character tables in IR and Raman spectroscopy.

Group theory and Quantum mechanics: wave functions as basis for irreducible representations, direct products, time-dependent perturbation theory, transition moment integral and selection rules in spectroscopy.

2. MICROWAVE SPECTROSCOPY **6+1 hours**

Rotations of molecules, ***rigid diatomic molecule-rotational energy expression, energy level diagram,*** selection rules, expression for the energies of spectral lines, computation of intensities, ***effect of isotopic substitution***, centrifugal distortion and the spectrum of a non-rigid rotor. Rotational spectra of polyatomic molecules - linear, and symmetric top molecules. Calculation of bond length of diatomic and linear triatomic molecules. Stark effect.

3. INFRARED SPECTROSCOPY **13+1 hours**

Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, fundamentals, overtones, hot bands, vibrational frequency, force constant, effect of isotopic substitution. Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules: Normal coordinate, translations, vibrations and rotations, vibrational energy levels, fundamentals, overtones and combinations. Vibration-rotation spectra of polyatomic molecules, parallel and perpendicular vibrations of linear and symmetric top molecules.

4. RAMAN SPECTROSCOPY 7+1 hours

Classical and quantum theories of the Raman effect, polarizability as a tensor, polarizability ellipsoids, relationship between applied electric field and polarizability, pure rotational Raman spectra of linear and symmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, elucidation of Raman activity using polarizability ellipsoids, rule of mutual exclusion, rotational fine structure – O and S branches. Polarization of Raman scattered photons. Structure determination from Raman and IR spectroscopy - AB_2 and AB_3 molecules.

5. ELECTRONIC SPECTROSCOPY 9 + 4 hours

Vibrational coarse structure, intensities by Frank-Condon principle, dissociation energy and dissociation products, rotational fine structure, Pre-dissociation.

Electronic structure of diatomic molecules-basic results of MO theory, Classification of states by electronic angular momentum, molecular orbitals, selection rules, spectra of singlet and triplet molecular hydrogen.

Application of group theory to the spectra of ethylene and benzene.

Decay of excited states-radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion (Jablonski diagram).

REFERENCES

1. Chemical Applications of Group Theory, 3rd edition, F.A. Cotton, Wiley Eastern (2009).
2. Introduction to Molecular Spectroscopy, C.N. Banwell and M.McCash, TMH Pub (2010).
3. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
4. Molecular Spectroscopy, J.D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
5. Modern Spectroscopy, J.M. Hollas, John Wiley (2010).
6. Vibrational Spectroscopy, D.N. Sathyanarayana, New Age International (P) Ltd. (1996).
7. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, (2001).

8. A simple approach to group theory in chemistry. S. Swarnalakshmi, T Saroja and R M Ezhilarasi. Universities Press. ISBN: 9788173716232, 9788173716232
9. Group Theory and Its Chemical Applications. ISBN: 9351428443, Himalaya Pub. House- New Delhi (2014)

Learning Outcomes: After learning this paper, students should be able to:

LO1	Knowledge	Define point groups, groups and subgroups, order, symmetry elements (identity, plane of symmetry, proper axis, improper axis, inversion center) and symmetry operations, harmonic and anharmonic oscillators and vibrational energy, rotational energy expression and its components, Frank-Condon principle, Born-Oppenheimer approximation, predissociation, dissociation energy in electronic states Write examples of conjugate relationships, classes of operations and order of a group, the great orthogonality theorem List the various symmetry elements for C_{2v}, C_{3v} and multiple higher-order axis symmetry operations in tetrahedral and octahedral point groups, properties of irreducible representations, the selection rules governing transitions in rotational, vibrational and Raman spectra Identify proper axis of symmetry, improper axis of symmetry and symmetry conditions for molecular chirality
LO2	Understand	Explain the fundamental concepts of symmetry elements and symmetry operations, and their representation in point groups using Schoenflies notations, inversion center, plane of symmetry, improper axis, the effect of isotopic substitution on the energy levels and rotational spectra, differences between electronic, vibrational, and rotational spectroscopy, band and progression in electronic transitions. Express Mulliken symbols for irreducible representations and their significance in characterizing molecular symmetry Compare the reducible and irreducible representations Compute characters of representations Summarize the concepts of fundamentals, overtones, and hot bands in vibrational spectroscopy.
LO3	Apply	Relate the polarizability ellipsoids to various vibrational modes, shape of the molecule to dipole moment and moment of inertia Determine point groups of molecules, the intensities of spectral lines based on transition between the rotational levels Construct irreducible representations of molecules (C_{2v} and C_{3v}) applying Great Orthogonality Theorem.

		Interpret the energy level diagrams for rotational transitions in diatomic molecules Predict the various Raman active/inactive modes with respect to polarizability ellipsoids of molecules, IR and Raman activity for various molecules using the character tables, rotational and vibrational spectral lines using Stark effect and nuclear spin effect to linear polyatomic and symmetric top molecules, relative intensities of spectral lines for transitions between the electronic energy levels. Solve structure of molecule (symmetric linear, asymmetric linear or bent) using the (PQR contour lines details- AB_2 and AB_3) Calculate bond lengths, frequencies of radiations absorbed during rotational, vibrational, and electronic transitions, rotational constants, moment of inertia, isotopic mass, force constants, bond dissociation energies of diatomic molecules Derive character tables for C_{2v} and C_{3v} point group using the corollaries of GOT Apply flow chart method to identify symmetry elements and operations in molecules Determine molecular parameters such as bond lengths and bond angles from spectral data Solve problems involving vibrational-rotational spectra of diatomic molecules, including the identification of P, Q, and R branches
LO4	Analyze	Compare molecular structures (AB_2 and AB_3) based on Raman vibrational modes, the spectrum of rigid and non-rigid rotor Compare and contrast the spectra of different diatomic molecules Analyze how molecular properties (bond strength, moment of inertia) affect the rotational spectra, vibrations of polyatomic linear molecules and symmetric top molecules using normal coordinates, Identify rotational transitions from spectral data
LO5	Evaluate	Compare dissociation energies calculated from equilibrium oscillation frequency and electronic spectral data.
LO6	Create	

Semester	I
Paper code	CH 7524
Paper title	PRINCIPLES OF CHEMICAL ANALYSIS
Number of teaching hrs per week	4
Total number of teaching hrs per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.

2. Text within parenthesis and italics correspond to recall/review**.**

1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION **13+1 hours**

***Significant Figures**:* (*Rounding of numbers. Addition and subtraction; multiplication and division.)*

Errors: Some important terms: replicate, outlier, accuracy, and precision. Errors affecting precision and accuracy; ***systematic errors*****:** ***sources and types of systematic errors with examples***. Ways of expressing accuracy: absolute and relative errors; constant and proportional errors. ***Detection of systematic instrument and personal errors***. Identification and compensation of systematic method errors. Terms used to describe the precision of a set of replicate measurements. Mean and median. Deviation and average deviation from the mean.

Statistical treatment of random errors; spread, sample, and population; sample mean and population means. Standard deviation and variance of population; Gaussian distribution. Propagation of determinate errors. Sample standard deviation, sample variance, standard error of the mean, relative standard deviation, coefficient of variation, pooled standard deviation. Statistical data treatment in scientific calculations. Confidence interval.

Student - t statistics, significance testing, null hypothesis, one-tailed and two-tailed significance tests. Comparing measured results with a known value.

Comparison of two experimental means. Comparison of standard deviation with F-test. Paired t-test for comparing individual differences. Error in hypothesis testing. Criteria for rejection of an observation- Q test, Grubbs's test. Quality assessment: control charts. Calibration curves: least square method. Finding the least square line. Expression for slope, intercept, standard deviation about regression. Standard deviation of the slope and intercept. Coefficient of determination. Calibration sensitivity, Analytical sensitivity, Linear dynamic range. Limit of detection (LoD) and limit of quantification (LoQ). Method validation, reporting analytical results.

2. ACID – BASE TITRATIONS **6+2 hours**

Basic principles: pH scale, dissociation constants of acids and bases. Titration curves for monobasic acids, pH calculations, theory of indicators. Titration curves for di, tri basic acids, amino acids, and bases. Fractions of phosphoric acid species as a function of pH. Gran's plots. Application of acid-base titrations for environmental, clinical, nutritional and industrial estimations.

Acid–base titrations in non-aqueous solvents –acid base window, acidic and basic titrants, methods of titration. ***Titrations in glacial acetic acid***, ***applications of non-aqueous titrations.***

3. REDOX TITRATIONS **7+1 hours**

Nernst equation, standard and formal potentials. Titration curves (calculations based on formal potentials), endpoint signals, indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent systems. Adjustment of analyte's oxidation state. ***Application of oxidants such as permanganate, dichromate, cerium (IV), bromates, iodates, and reductants such as ferrous ammonium sulphate and ascorbic acid***. Application for environmental, clinical, nutritional and industrial estimations.

Karl-Fischer titrations: Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds such as alcohols, carboxylic acids, acid anhydrides and carbonyl compounds.

4. PRECIPITATION TITRATIONS **4 hours**

Solubility product. Theoretical principles: titration curves, end point signals, Mohr, Volhard and adsorption indicators. Applications of argentometric titrations in estimation of F^-, K^+ and mixture of halides.

5. COMPLEXOMETRIC TITRATIONS **6+1 hours**

Complexometric titrations involving monodentate and polydentate ligands, advantages of EDTA. Expressions for the different fractions of EDTA in solution as a function of pH, conditional stability constants, effect of pH and second complexing agent on the conditional stability constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, application of EDTA titrations for environmental, clinical, nutritional and industrial estimations.

6. GRAVIMETRIC ANALYSIS **3+1 hours**

Types of gravimetric analysis, different steps involved in gravimetric estimation. Formation and treatment of precipitates, factors determining successful precipitation, nucleation and size of the particles, properties of precipitating agents. Coagulation and peptization. Von Weimarn's theory of relative supersaturation. Impurities in precipitates, co-precipitation, post precipitation. Methods of minimizing co-precipitation. Precipitation from homogeneous solution. Gravimetric factor. ***Important precipitating agents and their significance in inorganic analysis. Advantages and disadvantages of organic precipitants.***

7. KINETIC METHODS OF ANALYSIS 4+1 hours

Equilibrium and kinetic methods. Classification of chemical kinetic methods. Rate laws, pseudo-first-order kinetics, Expression for pseudo-first-order kinetics, types of kinetic methods, Direct computation and curve fitting methods. One-point and two-point fixed time integral methods for the calculation of rate constant. Direct computation variable time integral methods. Differential reaction rate methods, initial rate methods. Enzyme catalysis, basis for substrate and enzyme determination. ***Applications of catalytic and non-catalytic kinetic methods.***

Fast kinetics methods: femto-chemistry, direct determination of transition states, pulse radiolysis.

8. ABSORPTION AND EMISSION TECHNIQUES 6+1 hours

Quantitative aspects of spectrochemical measurements. (*Absorbance, molar absorptivity)*. Nephelometric and turbidimetric methods, choice of method and instrumentation. ***DU Pont model of turbidimeter, EEL nephelometer***. Analytical applications - turbidimetric titrations.

Molecular luminescence- explanation for fluorescence and phosphorescence using Jablonski diagram

Quantitative aspects of fluorescence. Variables that affect fluorescence and phosphorescence. Transition types in fluorescence. Fluorescence and structure, examples, effects of structural rigidity, temperature, dissolved oxygen and solvent. Effect of substitution on the benzene ring and fluorescence efficiency.

Atomic absorption methods: ***principle and instrumentation (single and double beam), light sources of AAS, atomization(flame and electrothermal),*** interferences in AAS and corrections applied. ***Atomic emission method (AES), advantages and disadvantages,*** Plasma – ICP, ICP sources, DCP, and ICP-MS techniques.

9. THERMAL METHODS OF ANALYSIS 3 hours

Introduction to thermal methods. Principle, instrumentation, data analysis and applications of thermogravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA) and thermometric titrations. Thermal analysis of polymers.

REFERENCES

1. Fundamentals of Analytical Chemistry, 10th Edn., D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, Cengage India Pvt. Ltd., 2023.
2. Principles of Instrumental Methods of Analysis,7thEdn., D. A. Skoog, F. J. Holler, S. R. Crouch, Cengage India Pvt. Ltd., 2020.

3. Analytical Chemistry; G. D. Christian, P. K. Dasgupta, K. V. Schug; Wiley India Pvt.Ltd., 2020.
4. Modern Analytical Chemistry, D. Harvey, McGraw Hill Higher education publishers, 2000.
5. Analytical Chemistry Principles,2^{nd} Edn., J. H.Kennnedy, Cengage Delmar Learning India Pvt.Ltd., 2011.
6. Quantitative chemical analysis, 10^{th} Edn., D. C. Harris, W. H. Freeman and Company, 2019.
7. Vogel's Textbook of quantitative chemical analysis, 6^{th}Edn.,J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Pearson Education Ltd., 2009.
8. Modern Physical Organic Chemistry, E. W. Anslyn and D. Dougherty, University Science Books, U.S., 2006.
9. Instrumental Methods of Chemical Analysis, V.K. Ahluwalia, Springer, 2023.
10. Chemical Analysis, 2^{nd}Edn., F. Rouessac, A. Rouessac, John Wiley & Sons Ltd, 2007.

Learning Outcomes: After learning this paper, students should be able to:

LO1	Knowledge	Recall: The concepts of gravimetric and volumetric analysis, significant figures and types of errors in chemical analysis, kinetics of different types of reactions, fundamental principles of analytical chemistry: pH scale, dissociation constants, titration curves, indicators, Nernst equation, standard and formal potentials, the principles of absorption and emission spectroscopy Define: co-precipitation, post precipitation, types of photophysical processes, conditional stability constant
LO2	Understand	Explain: the principle of chemical analysis and least-squares method, figures of merits in chemical analysis, different methods to minimize errors the kinetic methods, enzyme-catalyzed reactions, and fast reactions, the advantages, and disadvantages of organic precipitants, principles of nephelometry and turbidimetry Differentiate: between co-precipitation and post precipitation, between absorption and scattering techniques, between nephelometry and turbidimetry, between equilibrium methods and kinetic methods

LO3	Apply	Examine: different statistical tests to justify the authenticity of obtained results during chemical analysis, the kinetic techniques to measure the rate of a chemical reaction, concepts of acid-base titrations to perform pH calculations and select appropriate indicators for titration experiments, concepts of redox titrations to perform formal potential calculation and select suitable oxidants and reductants for titration experiments, Determine: the concentration of metal ions in a sample from gravimetric principles, various methods of titrations for environmental, clinical, nutritional and industrial estimations
LO4	Analyze	Analyze: the obtained data by subjecting them to different statistical treatments such as t-test, z-test, F-test, Q-test and Grubbs' test, different radiochemical techniques, in which the rate of nuclear decay of a radioactive element is measured Interpret:the titration curves and end point signals, unknown concentrations of a given experimental data, absorption and emission spectra in terms of molecular structure and composition Predict:the feasibility of redox reactions and the selection of appropriate indicators for redox titrations. Compare and contrast: different methods of volumetric and gravimetric analysis and their suitability for specific analytes and systems
LO5	Evaluate	Assess: the experimental data after performing hypothesis tests and decide whether to reject or accept the results obtained, the accuracy and precision of experimental results obtained from acid-base, redox, precipitation, and complexometric titrations Compare: different kinetic methods of chemical analysis including flow injection method. Evaluate: the advantages and disadvantages of different titration methods and techniques in analytical chemistry, predict the behavior of different analytes in gravimetric analysis, the limitations and assumptions of absorption and emission techniques in various analytical applications
LO6	Create	Design: a protocol to validate the analytical results obtained from an instrument and publish the result with all the necessary information, protocols for using absorption and emission techniques to analyze complex samples or investigate specific chemical phenomena Revise: methods and protocols to determine the concentration of

		acids, bases, oxidants, reductants, metal ions, and other substances using volumetric and gravimetric analysis

PRACTICALS

Semester	I
Paper code	CH7P1
Paper title	INORGANIC CHEMISTRY PRACTICAL I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

QUALITATIVE ANALYSIS: **11 sessions**

Semi-micro qualitative analysis of a mixture containing two cations and anions each and one rare element (W, Mo, Ce, Th, Zr, V, U and Li).

1. Explanation of acid radicals and model salt –acid radical analysis. (1 session)
2. Explanation of basic radicals and model salt – basic radical analysis. (1 session)
3. Salt mixture 1 (2 sessions)
4. Salt mixture 2 (1 session)
5. Salt mixture 3 (1 session)
6. Salt mixture 4 and RBPT (1 session)
7. Salt mixture 5 and RBPT (1 session)
8. Salt mixture 6 and RBPT (1 session)
9. Salt mixture 7 and RBPT (1 session)
10. Salt mixture 8 and RBPT (1 session)

REFERENCES

1. Vogel's Textbook of Qualitative Chemical Analysis, J Bassett, R C Denny, G H Jeffery and J Mendham, ELBS, 1986.
2. Vogel's Textbook of Quantitative Chemical Analysis, G N Jeffery, J Bassett, J Mendham and R C Denny, 5th edition Longman Scientific and Technical , 1999.
3. Inorganic semimicro Qualitative Analysis, V.V. Ramanujam, The National Publ. Co.,1974.

Learning Outcomes:

After performing these experiments, students will be able to:

LO-1	Remember	Differentiate the various radicals present in salt mixtures including rare cations.
LO-2	Understand	Explain the concept of solubility product and common ion effect.
LO-3	Apply	Perform analysis of cations and anions in a salt mixture samples.
LO-4	Analyze	Perform analysis of salt mixture samples containing more number of cations and anions Practice strict safety protocols, understand the handling of hazardous chemicals.
LO-5	Evaluate	Compare systematic analysis with spot tests.
LO-6	Create	Develop a protocol to do qualitative and quantitative analysis of given samples containing cations and anions.

Semester	I
Paper code	CH7P2
Paper title	INORGANIC CHEMISTRY PRACTICAL II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

II. QUANTITATIVE ANALYSIS: **11 Sessions**

1. Volumetric and gravimetric determination of the following mixtures:

(i) Iron and Aluminium– 2 sessions

(ii) Copper and Nickel – 2 sessions

(iii) Copper and Iron– 2 sessions

(iv) Copper and Zinc– 2 sessions

(v) Calcium and Barium– 2 sessions

2. Any other relevant experiment/ Viva -1 session

REFERENCES

1. Vogel's Textbook of quantitative chemical analysis, 6th Edn., J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Pearson Education Ltd., 2009.
2. Advanced Practical Chemistry, 2nd Edn., J. Singh, L. D. S. Yadav, R. K. P. Singh, I, R. Siddiqui, J. Singh, J. Srivastava, Pragati Prakashan, 2010.
3. Experimental Inorganic/Physical Chemistry, M. A. Malati, Woodhead Publishing Limited, 1999.
4. Practical Skills in Chemistry 3rd Edn., J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers, A. Jones, Pearson Education Limited, 2017.
5. Laboratory safety for chemistry students, 2nd Edn., R H. Hill, D. C. Finster, John Wiley & Sons, 2016.

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

LO1	Knowledge	Recall the laboratory safety precautions for a given experiment the principles of gravimetric and volumetric analyses, the stoichiometry and equations used in gravimetric and volumetric calculations, Record the details of an experiment performed.
LO2	Understand	Explain the theoretical principles behind gravimetric and

		volumetric methods for quantitative analysis. Understand the techniques involved in quantitative estimations based on volumetry and gravimetry.
LO3	Apply	Perform gravimetric and volumetric estimations of given sample applying the basic principles. Calculate the amount of the analytes present in a given mixture.
LO4	Analyze	Interpret the results obtained from gravimetric and volumetric experiments. Identify the potential sources of errors in gravimetric and volumetric experiments.
LO5	Evaluate	Assess the precision and accuracy of the quantitative estimations of analytes in a mixture.
LO6	Create	Design methods/protocols for the quantitative estimation of two cations/ anions using gravimetry and volumetry.

Semester	I
Paper code	CH 7P3
Paper title	ORGANIC CHEMISTRY PRACTICAL I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

QUALITATIVE ANALYSIS: 11 Sessions

Separation, systematic analysis and identification of organic compounds in a binary mixture.

1. Model mixture (1 Session)
2. Binary mixture 1 (2 Sessions)
3. Binary mixture 2 (2 Sessions)
4. Binary mixture 3 (1 Session)
5. Binary mixture 4 (1 Session)
6. Binary mixture 5 (1 Session)
7. Binary mixture 6 (1 Session)
8. Binary mixture 7 (1 Session)
9. Viva/repetition (1 Session)

REFERENCES

1. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari, 1996.
2. Practical Organic Chemistry, Mann and Saunders, 1980.
3. Textbook of Practical Organic Chemistry, A.I. Vogel, 1996.
4. Textbook of Quantitative Organic Analysis, A.I. Vogel, 1996.
5. A Handbook of Organic Analysis, Clarke and Hayes, 1964.

Learning Objectives

After performing these experiments, students will be able to:

LO1	Knowledge	Recall the principles, techniques, and systematic analysis procedures used in qualitative analysis of organic compounds from binary mixtures, including separation methods and chemical tests Recognize the importance of safety protocols and the significance of

		qualitative analysis techniques in diverse applications within organic chemistry research and industry contexts
LO2	Understand	Explain the principles and procedures involved in qualitative analysis, including separation techniques and chemical tests for identifying organic compounds
LO3	Apply	Apply separation techniques, systematic analysis procedures and qualitative tests to effectively separate and identify organic compounds within binary mixtures
LO4	Analyze	Analyze the effectiveness of separation techniques and systematic analysis procedures in isolating and characterizing organic compounds in the given binary mixtures, considering their advantages, limitations and trends in test results
LO5	Evaluate	Assess the overall credibility and significance of qualitative analysis results, including experimental data and problem-solving approaches Assign the functional group to the compound analyzed and confirm by preparing the derivative and taking melting point of the derivative
LO6	Create	Create innovative strategies, protocols, and frameworks for optimizing qualitative analysis procedures, including separation techniques and systematic qualitative analysis of organic molecules

Semester	I
Paper code	CH 7P4
Paper title	ORGANIC CHEMISTRY PRACTICAL II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Quantitative Analysis : 11 Sessions

1. Determination of equivalent weight of carboxylic acids. (1 session)
2. Saponification value of oil/fat. (1 session)
3. Estimation of glucose. (1 session)
4. Estimation of phenols by acylation method. (1 session)
5. Iodine value of oil/fat (1 session)
6. Estimation of glucose and sucrose in a mixture (1 session)
7. Estimation of acetone by Iodometry. (1 session)
8. Determination of amine salts by titration in aqueous solutions (1 session)
9. Estimation of nitro group. (1 session)
10. Estimation of nitrogen Kjeldhal's method. (1 session)
11. Estimation of carbonyl group by hydroxylamine-pyridine method. (1 session)
12. Any other relevant experiments / RBPT

REFERENCES

1. Laboratory Manual of Organic Chemistry, Day, Sitaramanand Govindachari, 1996.
2. Practical Organic Chemistry, Mannand Saunders,1980.
3. Textbook of Practical Organic Chemistry, A.I.Vogel 1996.
4. Textbook of Quantitative Organic Analysis, A.I.Vogel 1996.
5. A Handbook of OrganicAnalysis , Clarke and Hayes 1964.

Learning Objectives

After performing these experiments, students will be able to:

LO1	Knowledge	Recall the principle of volumetric titration for quantitative analysis, chemical reaction involved in the detection of glucose using Fehling's reagent, acid-base reactions and the concept of equivalent weight.

		List the reagents and equipment required for the quantitative analysis of organic compounds.
LO2	Understand	Describe the reactions involved during volumetric titration. Detail the concept of iodine value/saponification value and its significance in lipid analysis. Explain the importance of calibration and standardization procedures in titration experiments.
LO3	Apply	Identify various reagents and suitable reaction conditions in the estimation of organic compounds. Apply titration techniques specific to acid-base reactions, including the selection of appropriate indicators, the determination of endpoints. Demonstrate proper handling of chemicals and equipment during the experiment. Apply appropriate calculations to estimate an organic compound.
LO4	Analyze	Identify the amount of organic compound present in a sample. Interpret saponification value/iodine value data to evaluate the quality of oils and fats.
LO5	Evaluate	Assess the feasibility of these methods in the estimation of structurally related organic compounds.
LO6	Create	Design the suitable method to estimate the amount of a given organic compound.

Semester	II
Paper Code	CH8124
Paper Title	INORGANIC CHEMISTRY – II
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.

2. Text within parenthesis and italics correspond to recall/review.

1. METAL – LIGAND BONDING **12+3 hours**

<u>Basic concepts of co-ordination chemistry</u>. Crystal field theory: crystal field splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal ligand fields; structural and thermodynamic effects of crystal field splitting; octahedral ionic radii, Jahn–Teller distortion in metal complexes and metal chelates, hydration and lattice energies, site preferences in spinels, octahedral versus tetrahedral co-ordination, Irving-William stability order; spectrochemical series; limitations of crystal field theory. Evidences for metal– ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling; nephelauxetic effect and nephelauxetic series. Ligand Field Theory, Ligand Group of Orbitals. MO theory: symmetry adapted linear combinations of Atomic Orbitals, MO diagrams of octahedral complexes (including π-bonding). ***<u>MO energy level diagrams in tetrahedral complexes</u>***.

2. METAL – LIGAND EQUILIBRIA IN SOLUTION **7+1 hours**

Step-wise and overall formation constants and their relationships, trends in step-wise formation constants and exceptions to the trends; factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macrocyclic effects and their thermodynamic origin; kinetic and thermodynamic stability of metal complexes.

<u>Determination of composition and stability constants of complexes by spectrophotometry (Job's method) and potentiometry.</u>

3. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 12+1 hours

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel and Tanabe-Sugano diagrams, Correlation diagram of d^2 configuration, spectra of 3d metal aqua complexes of trivalent V, Cr, divalent Mn, Co, Ni, and $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra, ***spectral behaviour of lanthanide ions***. Introduction to emission spectrum, emission spectra of lanthanides (Eu^{3+} and Tb^{3+}).

4. MAGNETIC PROPERTIES OF METAL COMPLEXES 9+1 hours

Origin and types of magnetic behaviour; diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method, Evans method, and ***SQUID***. Temperature dependence of magnetism – Curie and Curie-Weiss laws, types of paramagnetic behaviour; temperature independent paramagnetism, spin-orbit coupling, magnetic behaviour of lanthanide ions, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), spin-cross over. EPR spectra of transition metal ion complexes: hyperfine splitting, zero field splitting and Kramer's degeneracy, interpretation of g-values. ***Applications of magnetic data***.

5. STRUCTURE AND BONDING IN SELECTED METAL COMPLEXES 12+2 hours

Hydride, dihydrogen, isocyanide complexes; mononuclear and dinuclear metal carbonyls and metal carbonyl clusters, ***Wade's rules as applied to metal carbonyl clusters***, nitrosyl, dinitrogen and tertiary phosphine and N-heterocyclic carbene complexes, Comparison of steric (cone angles vs % buried volume) and electronic parameters between tertiary phosphine and N-heterocyclic carbenes).

Stereochemical non-rigidity, Stereoisomerism – chirality, optical activity, Circular Dichroism, Optical Rotatory Dispersion, Cotton effect and absolute configurations.

Concepts of Supramolecular Chemistry: Definition, nature of supramolecular interactions, host-guest interaction, molecular recognition, types of recognition, self-assembly.

Cation-binding Hosts: Concepts, cation receptors, ***crown ethers, cryptands, spherands, calixarenes***, selectivity of cation complexation, template effect.

REFERENCES

1. Inorganic Chemistry, 5th Edn., C. E. Housecraft and A. G. Sharpe, Pearson Education Ltd., 2018.
2. Inorganic Chemistry, 7th Edn., M. Weller, J. Rourke, T. Overton and F. Armstrong, Oxford Univ. Press., 2018.
3. Advanced Inorganic Chemistry, 6th Edn., F. A Cotton and G. Wilkinson, John Wiley & Sons Inc., 1999.

4. Advanced Inorganic Chemistry, 3rd Edn., F. A. Cotton and G. Wilkinson, Wiley Eastern limited, 1972.
5. Inorganic Chemistry, 4th Edn., J. E. Huheey, E. A. Keiter and R. L. Keiter, Pearson Education Asia Pvt. Ltd., 2000.
6. Foundations of Inorganic Chemistry, G. Wulfsberg, University Science Books, 2018.
7. Physical Methods in Inorganic Chemistry, R. S. Drago, Von Norstand compounds, 1965.
8. Inorganic Chemistry, 5th Edn., G. L. Miessler, P. J. Fischer, D. A. Tarr, Pearson Education Ltd., 2014.
9. Theoretical Inorganic Chemistry, M. C. Day and J. Selbin, Litton Educational Publishing Inc., 1969.
10. Coordination Chemistry, 2nd Edn., D. Banerjea, Asian Books Pvt. Ltd., 2007.

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

LO1	Knowledge	Recall the terms, concepts, rules, theorems, relationships, classifications, geometries, orbital splitting patterns, ligand sequences and energy level diagrams pertaining to metal-ligand (M-L) bonding, thermodynamic stability, spectral and magnetic properties of metal complexes. Write limitations of crystal field theory, origin and types of magnetic behaviour, Curie and Curie-Weiss laws, factors affecting the stability of metal complexes, term symbols for d^n ions and their significance in determining electronic configurations, selection rules governing electronic transitions in transition metal complexes, Define kinetic and thermodynamic stabilities of metal complexes
LO2	Understand	Explain crystal field splitting in various ligand fields, structural and thermodynamic effects of d-orbital splitting, evidences for M-L covalent bonding, LCAOs, bonding/properties of complexes based on MO theory, factors affecting stability of complexes Describe the determination of stability constants, structure/ bonding in different types of coordination complexes Discuss types of paramagnetic behaviour, temperature independent paramagnetism, spin-orbit coupling, magnetic behaviour of lanthanide ions, quenching of orbital contribution and spin only behaviour, spin-cross over, EPR spectra of transition metal ion complexes: hyperfine splitting, zero field splitting and Kramer's degeneracy, stereochemical non-rigidity, stereoisomerism, chirality, optical activity, CD,

		ORD, Cotton effect Differentiate between stepwise and overall stability constants, kinetic and thermodynamic stability
LO3	Apply	Calculate 10 Dq and β values from Tanabe- Sugano diagrams, CFSE, stabilization due to tetragonal distortion, octahedral site preference energy in spinels and OSSE in complexes, magnetic moments, overall stability constants Predict polyhedral structure of multinuclear polymetallic carbonyl clusters, relative stabilities of complexes Assign the absolute configuration of complexes using CD, ORD data Construct Orgel and Tanabe-Sugano diagrams for transition metal complexes and assign electronic transitions Interpret the structural and thermodynamic aspects of metal complexes using CFT and MOT, the deviation of magnetic moments from spin-only value, the structural information from spectral data and magnetic measurements
LO4	Analyze	Predict the possibility of Jahn-Teller distortion in different d^n configurations, preference for octahedral/tetrahedral geometry in complexes, spinel structures Compare steric and electronic properties of phosphine and NHC ligands Compare and contrast modern theories of bonding in the interpretation of the structures and properties of metal complexes
LO5	Evaluate	Assess the effectiveness of CFT and MOT in interpreting the structures and properties of complexes Evaluate the effectiveness of Orgel and Tanabe-Sugano diagrams in predicting electronic transitions in transition metal complexes.
LO6	Create	Validate the structures of a given complexes from spectral data and magnetic studies.

Semester	II
Paper Code	CH8224
Paper Title	ORGANIC CHEMISTRY – II
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. ADDITION REACTIONS (8+2) hours

Addition to carbon-carbon multiple bonds: ***<u>General mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity</u>***; hydrogenation and hydroboration; Nucleophilic addition: Michael addition, mechanisms of formation of hydrates, acetals, oximes and hydrazones of carbonyl compounds, Wittig reaction.

Addition to carbon-heteroatom multiple bonds: mechanisms of metal hydride reduction of carbonyl compounds and nitriles. ***<u>Addition of Grignard reagents and organolithium reagents to carbonyl compounds</u>***

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION (4+1) hours

S_E1, S_E2 and S_Ei mechanisms, hydrogen exchange, migration of double bonds. Aliphatic diazonium coupling, nitrosation at carbon and nitrogen, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids; Haller-Bauer reaction.

<u>Halogenation of aldehydes, ketones and acids, haloform reaction</u>**.**

3. REARRANGEMENTS 14+1 hours

Carbon to carbon migrations: ***<u>Wagner-Meerwein, pinacol-pinacolone</u>***, benzil-benzilic acid, Favorskii and Neber rearrangements; Arndt-Eistert synthesis; expansion and contraction of rings.
Carbon to nitrogen migrations: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.
Nitrogen/oxygen/sulfur to carbon migrations: Stevens and Wittig rearrangements.
Carbon to oxygen migrations: Baeyer-Villiger rearrangement.
Non-1,2 rearrangements: Fischer indole synthesis, benzidine rearrangement.

4. PERICYCLIC REACTIONS (17+3) hours

Molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene. Meaning of HOMO, LUMO, bonding, antibonding and nonbonding molecular orbitals.

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems; classification of pericyclic reactions. Theories to rationalize pericyclic reactions: Frontier Molecular Orbital approach (FMO), Woodward-Hoffmann orbital Symmetry Correlation Diagram, Woodward-Hoffmann rules, Hückel-Mobius (perturbation molecular orbital or transition state aromaticity) method.

Electrocyclic reactions: conrotatory and disrotatory modes; 4n, 4n+2 and allyl systems, torquoselectivity. Cycloadditions: suprafacial and antarafacial additions, 4n and 4n+2 systems; Diels-Alder reactions: Normal and inverse electron demand, Relative reactivity of dienes, regioselectivity, Alder Endo rule, hetero- and retro-Diels-Alder reactions. Trapping of reactive intermediates by Diels-Alder reactions. [2+2] addition of ketenes, 1,3-dipolar cycloadditions: ***application in click chemistry and bio-orthogonal chemistry.*** Cheletropic reactions involving carbene, CO, SO_2, and diazene.

Sigmatropic rearrangements: Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5-, 3,3-, 5,5- and 2,3-sigmatropic rearrangements; Cope, oxy-Cope and Claisen rearrangements; Sommelet-Hauser rearrangement.

Group transfer reactions: Alder-ene reaction, Metallo-ene reaction.

Application of pericyclic reactions in Vitamin-D synthesis.

5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY (9+1) hours

Generation of free radicals via hydrogen abstraction and chain process.

(Free radical addition, substitution, elimination, rearrangement and electron transfer reactions).

Use of free radicals in organic synthesis.

General principles of photochemistry: (*singlet and triplet states-differences in reactivity, photosensitisation; quantum yields)*.

Triplet-triplet annihilation, delayed fluorescence.

Photochemical reactions: Norrish type I and type II cleavages, cis-trans isomerization of stilbene, di-p-methane rearrangement; Paterno-Buchi reaction; photoreduction of ketones; photochemical oxidations: photosensitization oxidation and photosensitized oxygen transfer, cycloaddition of singlet molecular oxygen. Photochemistry of arenes. ***Photo Fries rearrangement,*** Hoffmann-Loeffler-Freytag reaction.

REFERENCES

1. March's Advanced Organic Chemistry, Michael B. Smith and J. March, 6th Edn., John Wiley, 2007.
2. Advanced Organic Chemistry, Part A and B, F. A. Carey and J. Sundberg, 5th Edn., Plenum press, 2007.
3. Organic Chemistry, Paula Yurkanis Bruice, 8th Edn., Pearson Education, Inc., 2020.

4. Organic Chemistry, J. Clayden, N. Greeves, S. Warren , 2nd Edn., Oxford University Press, 2012.
5. Molecular orbitals and Organic chemical reactions, Ian Fleming, John Wiley, 1st Edn, 2010.
6. Organic Photochemistry, J.M. Coxon and B. Halton, Cambridge India, 2nd Edn, 2015.
7. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry and Kathleen S. Richardson, Pearson, 3rd Edn, 1997.
8. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, S. Sankararaman, Wiley VCH, (2005).
9. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, 5th Edn. New Age International Publishers, 2023.
10. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy and J.C. Scaiano, University Science Books, 2010.
11. Pericyclic Reactions, S. Kumar, V. Kumar, and S. P. Singh, Academic Press, 2016.
12. Modern Physical Organic Chemistry, E. W. Anslyn and D. Dougherty, University Science Books, U.S., 2006.
13. Photochemistry of Organic Compounds, Petr Klan and J. Wirz, 1st Edn, John Wiley and Sons Ltd., 2009.

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

LO1	Knowledge	Recall the nucleophilic, electrophilic addition reactions; the generation of free radicals and organic reactions involving free radicals; the general principles of photochemistry; the general types of rearrangement reactions Define pericyclic reactions
LO2	Understand	Explain the driving forces and factors influencing addition and rearrangement reactions; basic concept of thermal and photochemical pericyclic reactions; the types and stereochemical aspects of important pericyclic and photochemical reactions; Draw the proposed mechanisms for the addition reaction and rearrangement reaction Discuss various types of photochemical reactions and their reaction mechanism
LO3	Apply	Assess the stereochemical outcome of an addition reaction concerning the number of new stereocentres/ racemate formation/ mixture of diastereomers. Predict the structure of the reaction products with correct stereochemistry under thermal and photochemical conditions;

		outcome of rearrangement reactions; key functional groups and understanding reaction mechanisms
LO4	Analyze	Point out whether an acid or a base can be used to catalyse a reaction. Compare and contrast between various types of photoinduced organic reactions; various rearrangement reactions in terms of their mechanisms, selectivity, and synthetic utility. Infer the steps involved in complex rearrangement reactions through key intermediates and transition states
LO5	Evaluate	Recommend suitable pericyclic reactions and starting materials to synthesize the target molecule. Decide reaction conditions that favour specific rearrangement reactions
LO6	Create	Design a synthetic route to prepare organic compounds for various applications through pericyclic reactions, addition, substitution and rearrangement reactions

Semester	II
Paper Code	CH 8324
Paper Title	PHYSICAL CHEMISTRY – II
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.
2. Text within parentheses and italics correspond to recall/review.

1. STATISTICAL THERMODYNAMICS **11 + 4 hours**

Introduction: Objectives of statistical thermodynamics, inputs from quantum mechanics and spectroscopy, system in terms of energy levels and population, thermally available energy levels, micro and macro states and their representation, distinguishable and indistinguishable particles, configuration and its weight, dominant configuration, ensemble and its types, ensemble averaging, postulates of statistical thermodynamics. Thermodynamic probability, its relationship with entropy. Stirling's approximation and Lagrange method of undetermined multipliers.

Introduction to quantum statistics. Different distribution laws and types of statistics. Maxwell-Boltzmann statistics: assumptions, derivation of equation for fraction of molecules occupying a given energy range, partition function and its physical significance. Bose-Einstein statistics: assumptions, <u>***derivation of equation for fraction of molecules occupying agiven energy range***</u>. Fermi-Dirac statistics: assumptions, <u>***derivation of equation for fraction of molecules occupying a given energy range***</u>. Comparison of Bose-Einstein and Fermi-Dirac statistics with Maxwell-Boltzmann statistics. Molar and molecular partition functions. Derivation of translational/rotational/vibrational/electronic partition functions. Relationship between partition function and thermodynamic parameters – internal energy, heat capacity, free energy, chemical potential, pressure, entropy and equilibrium constant. Sackur-Tetrode equation. Evaluation of partition functions from spectral data, thermodynamic properties of molecules from partition functions. <u>***Application of statistical thermodynamics: equipartition theorem, heat capacity behavior of crystals.***</u>

2. CHEMICAL THERMODYNAMICS **15 hours**

Introduction – review of thermodynamic laws and their significance.

Thermodynamics of open systems, partial molal quantities: partial molal free energy, partial molal volume. Determination of partial molal volume: graphical methods, intercept method (reciprocal density method and mole fraction) and apparent molar volume method. Gibbs-Duhem equation. Chemical potential and its significance, effect of temperature and pressure on chemical potential, chemical potential of a pure substance, ideal gas mixture and liquid mixture. Fugacity, determination of fugacity by graphical method and compressibility factor method, variation of fugacity with temperature and pressure.

Activity and activity coefficients: determination by solubility and emf methods, effect of temperature and pressure on activity. Gibbs-Duhem-Margules equation – derivation and applications; Konovalov's first law and second law.

Thermodynamic deduction of Henry's law, Raoult's law, Nernstdistribution law, Phase rule and their validation using chemical potential. Thermodynamics of mixing of ideal solutions and non-ideal solutions. Excess thermodynamic functions.

3. NON-EQUILIBRIUM THERMODYNAMICS 8 hours

Irreversible processes and steady state. Conservation of mass and energy in open systems. Fluxes andforces Entropy production – entropy production due to heat flow. Entropy production and it's rate in matter flow. Microscopic reversibility and Onsagar's reciprocity relations. Phenomenological equations. Entropy production in terms of fluxes and forces. Entropy production and its rate in chemical reactions.

4. REACTION KINETICS 16 + 2 hours

Arrhenius and bimolecular collision theories. Activated complex theory – derivation of expression forrate constant by thermodynamic method and partition function method. Reactions in solutions – factors affecting reaction rates in solutions.

Diffusion controlled reactions – influence of solvation, internal pressure and dielectric constant on reaction rates. Ionic reactions – double sphere model for effect of solvent on ionic reaction rates. Diffusion controlled reactions.

Primary and secondary salt effects.

Kinetic and thermodynamic control of reactions.

Unimolecular reactions – quantitative treatment of Lindemann and Hinshelwood theories, qualitative treatment of RRK and RRKM theories, comparison of these theories.

Kinetics of chain reactions – H_2 and O_2 reaction – Explosion limits. Dehydrogenation of ethane, pyrolysis of acetaldehyde - Rice - Herzfeld mechanisms.

Kinetics of fast reactions, features of fast reactions.

Study of fast reactions by flow method, relaxation method, flash photolysis and NMR method.

5. KINETICS OF POLYMERIZATION 4 hours

Kinetics and mechanism of free radical polymerization, kinetic chain length and chain transfer. Kinetics of cationic and anionic polymerization. Co-polymerization – free radical mechanism, copolymer composition.

REFERENCES

1. Physical Chemistry, P.W. Atkins, Julio de Paula, 9th Edn., W.H. Freeman and company, 2010.

2. Chemical Kinetics, K. J. Laidler, 3rd Edn., Pearson Education, Singapore, 2004
3. Advanced Physical Chemistry, J. N. Gurtu and A. Gurtu, 8th Edn., Pragati Prakashan, 2006.
4. Textbook of Physical Chemistry, H. K. Moudgil, PHI Learning Pvt. Ltd., New Delhi, 2010.
5. Principles of Physical Chemistry, B.R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishersco, 2017.
6. Molecular thermodynamics, Donald A. McQuarrie, John D. Simon UniversityScience Books, California, 1999.
7. Polymer Science, V. R. Gowarikar, N. V. Viswanathan and J. Sreedhar, 1st Edn., New age International (P)Ltd. Publishers. First edition, 2012.
8. Thermodynamics, Rajaram and J. Kuriacose, Shobhanlal Publishers, 1999.

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

LO1	Knowledge	**Recall:** principles of non-equilibrium thermodynamics, irreversible processes, steady-state conditions, and conservation laws for mass and energy in open systems. **Identify:** entropy production's significance in understanding irreversible processes, ensemble average and principle of equal a priori probability. **State** the linear law and express heat transfer. **Describe** postulates of irreversible thermodynamics. **Identify** conjugate fluxes and forces. **Define** i) primary and secondary salt effects ii) diffusion-controlled reaction. **Recall** equations from activated complex theory for rate constants calculation. **Describe** i) reaction kinetics theories: Arrhenius and bimolecular collision ii) cationic, anionic, and co-polymerization iii) partial molal volume, free energy, chemical potential, activity, coefficient, fugacity, and excess thermodynamic functions iv) the relationship between partial molal volume and solute behavior v) the significance of partition functions, **List** i) factors affecting reaction rates in solutions. Write chain length expression for chain reactions kinetics ii) salient features of RRK and RRKM theories iii) effective catalysts for cationic polymerization. **Define** Gibbs-Duhem, Gibbs-Duhem-Margules, Konovalov's I and II laws. **Explain** i) the significance of chemical potential, activity, and fugacity ii) the relationship between statistical and classical thermodynamics. **Write** expressions for i) chemical potential, ii) mean activity, iii) mean activity coefficient, iv) ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, ΔH_{mix} for ideal and non-ideal solutions v) thermodynamic probability vi) partition functions (translational, rotational, vibrational), and law of equipartition energy, vii) internal energy, heat capacity, entropy, enthalpy, work function, and Gibbs free energy in terms

		of partition functions. **Define** microstates, macrostates, ensembles, partition function, Boltzmann distribution, and statistical mechanics. **List** assumptions/features for Bose-Einstein, Maxwell-Boltzmann, Fermi-Dirac distributions.
LO2	Understand	**Explain:** i) the relationship between fluxes and forces in non-equilibrium systems and their contribution to entropy production ii) the postulates of irreversible thermodynamics iii) steady state with relevant examples iv) the concept of microscopic reversibility and its implications in Onsager's reciprocity relations iv) the principle of flash photolysis v) relaxation methods vi) the mechanisms for chain reactions vii) the Rabinowitch effect v) the influences of solvation, internal pressure, and dielectric constant on diffusion-controlled reactions, and effects of solvent on ionic reaction rates using the double sphere model. **Identify:** i) the forces and fluxes involved in the polymerization of isobutene with water and BF_3, ii) the free radical propagation mechanism and propagation rates in co-polymerization iii) how chemical potential varies with changes in temperature and pressure iv) molecular and molar partition functions. **Discuss:** i) the salient features of RRK and RRKM theory ii) reasons for the first and second explosion limits in gas-phase combustion reactions iii) application of phenomenological equations in describing non-equilibrium thermodynamic phenomena iv)activated complex theory and its application in predicting reaction rates v) conditions for explosion and explosion limits vii) comparison between cationic and free radical polymerization vii) thermodynamics of mixing for ideal and non-ideal solutions. **Describe** the principles underlying the Arrhenius equation and how they relate to reaction rates and temperature. **Calculate** probability distributions used in statistical thermodynamics (Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac). Distinguish between: Thermal equilibrium and steady-state, Fermi-Dirac and Maxwell-Boltzmann statistics, Fermi-Dirac and Bose-Einstein statistics, Maxwell-Boltzmann sand Bose-Einstein statistics.
LO3	Apply	**Apply:** i) the principles of non-equilibrium thermodynamics to analyze and solve problems related to entropy production in various physical and chemical systems ii) Brønsted-Bjerrum equation to explain the influence on rate if ionic charges and or the nature of the electrolyte is specified. iii) steady-state model and derive an expression for the overall formation of the product in the case of chain reactions iv) theory to predict the reaction rate on increasing the charge v) a steady-state hypothesis to predict the order of the reaction at

		low and high pressures if the mechanism of unimolecular reactions is given vi) Rice and Herzfeld mechanism for the kinetics of decomposition of acetaldehyde and ethane, vii) the conditions for the explosion and the explosion limits for the reaction between hydrogen and oxygen viii) quantitative and qualitative treatments of unimolecular reactions by Lindemann, Hinshelwood, RRK, and RRKM theories ix) Gibbs-Duhem-Margules equation to prove that in a binary solution if the solvent obeys Raoult's law then the gas obeys Henry's law x) Konovalov's laws to explain the principles of fractional distillation xi) chemical potential to validate phase rule xii) the partition function to compute thermodynamic properties of systems, such as internal energy, entropy, and free energy xiii) the concepts of partition function for different types of systems, including monoatomic and diatomic, xiv) the concept of partition function to explain Einstein's theory of heat capacity. **Construct** phenomenological equations for a process involving more than two fluxes and forces. **Prove** that the energy received by subsystem I from subsystem II is equal and opposite sign to that received by system II from I through the thermallyconducting surface. **Derive** an expression for entropy production i) in terms of fluxes and forces ii) in heat flow iii) matter flow and iv) in chemical reactions **Explain** kinetics of polymerization and by using radical mechanism and applying steady state. **Predict** i) the products based on the structure of the activated complex, extent of solvation, and effect on activity coefficient ii) the partition functions for a system containing a monoatomic gas iii) and interpret experimental results by applying the knowledge of primary and secondary salt effects. **Prove** that a loose vibrational motion ultimately gets converted to a translational motion. **Evaluate** the diffusion-controlled rate constant for the reaction between two molecules **Calculate:** the i) fraction of molecules having sufficient energy to react and form the product if activation energy for a reaction is given, along with the number of collisions ii) ionic strength of a solution iii) $\Delta^{\#}G^0$, $\Delta^{\#}H^0$, $\Delta^{\#}S^0$, and the pre-exponential factor for the reaction from the given data of rate constant, Ea, and T iv) the partial molal volume v) Calculate ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, and ΔH_{mix} for ideal and non-ideal solutions, vi) excess thermodynamic properties (G^E, S^E, H^E, V^E, and μ^E) vii) the nuclear partition function of the ortho hydrogen and para-hydrogen molecules viii) the translational partition function, rotational partition function andvibrational partition function. **Choose** the solvents in the increasing order of reaction rate between a pairof ions and explain the order of the arrangement. Formulate an expression for the consumption of a monomer.

		Derive: i) an expression for the rate constant using conventional transition state theory by treating the motion over the energy barrier as a loose vibrational ii) an expression for the rate constant using conventional transition state theory by treating the motion over the energy barrier as translational iii) thermodynamic formulation of conventional transition state theory and obtain an expression for the rate constant of an unimolecular reaction iv) an expression for rate constant and discuss the effect of internal pressure on reaction rates v) Henry's, Raoult's and Nernst distribution laws from chemical potential vi) an expression for apparent molar volume vii) ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, and ΔH_{mix} for ideal and non-ideal solutions viii) Gibbs-Duhem equation ix) Gibbs-Duhem-Margules equation x) Konovalov's I and II law from Gibbs-Duhem-Margules equation xi) Sackur-Tetrode equation to determine translational entropy of a monoatomic gas xii) translational partition function, rotational partition function and vibrational for a monoatomic gas xiii) the expression for the distribution of particles using Maxwell-Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics xiv) relationship of the partition function with internal energy, entropy, Gibbs free energy, work function and enthalpy xv) an expression for equilibrium constant (K_p) in terms of partition functions, xvi) law of equipartition energy using partition function. **Determine:** i) activity and activity coefficient using emf and solubility measurements, ii) partial molal volume using reciprocal density method iii) partial molal volume using intercept method when mole fractionis given. Explain the effect of variation of temperature and pressure on chemical potential.
LO4	Analyze	**Analyze:** i) the factors influencing entropy production in different processes,such as heat flow, matter flow, and chemical reactions ii) the kinetics of chain reactions, such as the H_2 and O_2 reactions, and interpret explosion limits, iii) mechanisms such as the Rice-Herzfeld mechanism in thedecomposition of a molecule and predict the order of the reaction iv) the given mechanism and propose the order of the reaction in the case of decomposition of an organic molecule, apply steady state, and evaluate activation energy v) the stated conditions to predict the explosion and the explosion limits for the reaction between any two reactants vi) and predict the rates of reactions from the given data on ionicstrength. **Compare and contrast** i) different theories of unimolecular reactions to understand their strengths and limitations ii) RRK and RRKM theories. **Predict:** i) the reaction rates based on dielectric constants' data of solvents ii) the effect of solvation on the reaction rate for any

		reaction based on the solvent polarity. **Choose** the solvents in the increasing order of reaction rate between a pairof ions and explain the order of the arrangement. **Infer** the kinetics of polymerization by applying steady state and using a free radical mechanism. Justify the reaction outcomes by applying the concepts of kinetic and thermodynamic control. **Identify** the decrease in volume of solution after mixing two solvents. Correlate the decrease in the volume for a mixture of liquids to partial molal property. **Examine** the scale-up ratio required to obtain the desired volume aftermixing two solvents using the principles of partial molal volume. **Relate** macroscopic properties of systems to its microscopic states. Compare and contrast the predictions of statistical mechanics with those of classical thermodynamics.
LO5	Create	**Develop:** strategies to control reaction kinetics for desired outcomes in chemical processes, considering factors such as temperature, concentration,and solvent properties. **Arrive** at the molecular spectra from statistical thermodynamics. Apply the concepts of partition function for polyatomic molecules.
LO6	Evaluate	**Evaluate:** i) the significance of entropy production as a measure of irreversibility in natural and engineered systems ii) the features and characteristics of fast reactions and their significance in chemical processes, iii) partition functions from spectral data. **Critically evaluate** the methods used to study fast reactions, including flow,relaxation, flash photolysis, and NMR methods, in terms of their strengthsand limitations. Analyze the given data of different reactions, plot it on ln (k/k_o) versus square root of ionic strength, and predict the effect on reaction rates. **Develop** strategies to control reaction kinetics for desired outcomes in chemical processes, considering factors such as temperature, concentration,and solvent properties. **Assess** the validity of statistical mechanics predictions by comparing with experimental observations.

Semester	II
Paper Code	CH8424
Paper Title	SPECTROSCOPY – II
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.

2. Text within parenthesis and italics correspond to recall/review.

1. UV AND VISIBLE SPECTROSCOPY 4+2 hours

Nature of electronic transitions; the origin of UV band structure; principles of absorption spectroscopy, instrumentation and presentation of spectra. Solvents; terminology: chromophores; auxochromes; bathochromic shift; hypsochromic shift, hyperchromic shift, hypochromic shift. Effect of conjugation on the spectra of alkenes. Woodward-Fieser rules for polyenes. Electronic spectra of carbonyl compounds. Effect of solvent on π–π^* and n–π^* transitions. Woodward's rules for enones.

2. INFRARED SPECTROSCOPY 6+2 hours

Infrared portion of electromagnetic spectrum. Energy, frequency, wave number relationship. Infrared absorption process. Principle of IR analysis, Uses of infrared spectrum. Modes of stretching and bending vibrations. Bond properties and absorption trends. Instrumentation of IR spectrometer: Dispersive and Fourier transform spectrometers. Preparation of samples for IR analysis. Analysis of an IR spectrum at a glance. Survey of functional groups with examples. Hydrocarbons: alkanes, alkenes and alkynes, aromatic hydrocarbons: Detailed discussions on C–H vibrations, C=C vibrations, conjugate effects and ring size effects (internal bonds) =C–H bending vibrations (in alkenes and aromatic compounds-discussion on substitution patterns). Alcohols and phenols, ethers: Detailed discussion on O–H stretching vibration, effect of hydrogen bonding (effect of solvent polarity and concentration). Carbonyl compounds: normal base values for C=O stretching vibrations for carbonyl compounds. Effect of electron withdrawing groups, inductive, resonance, hydrogen bonding, conjugation, ring size. General discussions of IR absorption characteristics of aldehydes, ketones, carboxylic acids, esters ketones and amides, acid anhydrides and chlorides. IR spectra of nitriles and phosphorous compounds, structure determination of simple molecules.

3. **NMR SPECTROSCOPY 17+1 hours**

Nuclear spin states; nuclear magnetic moments; absorption of energy; mechanism of absorption (resonance). Population densities of nuclear spin states; the chemical shift and shielding; Instrumentation of nuclear magnetic resonance spectrometer-continuous-wave (CW) and pulsed fourier transform (FT) instrument. Chemical equivalence; integrals and integration; chemical environment and chemical shift; local diamagnetic shielding-electronegativity effects; hybridization effects; acidic and exchangeable protons; hydrogen bonding. Magnetic anisotropy; spin–spin splitting (n+1) rule; origin of spin-spin splitting; Pascal's triangle. Low- and high-resolution spectra of ethanol-chemical exchange; NMR spectra of amides. Coupling constant; solving NMR spectra problems. Coupling constants: mechanism of coupling-one-bond couplings (^{1}J); two-bond couplings (^{2}J); three-bond couplings (^{3}J)-Karplus relationship. Long-range couplings (^{4}J-^{n}J); magnetic equivalence. Use of tree diagrams when the n+1 rule fails; measuring coupling constants from first-order spectra. Second-order spectra-strong coupling; Pople notation for spin systems.

4. CARBON–13 NMR SPECTROSCOPY **7 hours**

Carbon-13 nucleus; carbon-13 chemical shifts; proton-coupled C-13 spectra-spin-spin splitting of carbon-13 signals. Proton-decoupled C-13 spectra; nuclear Overhauser effect. Cross-polarization: origin of the nuclear Overhauser effect; problems with integration in C-13 spectra. Molecular relaxation processes; off-resonance decoupling.

5. ADVANCED NMR TECHNIQUES **4+1 hours**

Pulse widths, spins, and magnetization vectors. DEPT experiment: number of protons attached to C-13 atoms; determining the number of attached hydrogens. Introduction to two-dimensional spectroscopic methods; COSY technique: ^{1}H-^{1}H correlations; HETCOR technique: ^{1}H-^{13}C correlations; an overview of COSY and HETCOR experiment. ***How to read COSY and HETCOR spectra.***

6. MASS SPECTROMETRY **6+2 hours**

Principle of mass spectrometry, mass spectrometer, resolution mass spectrum, molecular ion peak, base peak, fragment ion peaks, meta stable ion peak, isotope peaks, Nitrogen rule - definition and their significance. Determination of molecular weight and molecular formula. Carbocation: stability, types of fragmentation patterns: single bond, multiple bonds, McLafforty rearrangement, retro Diels-Alder. General discussions on the fragmentation patterns of alkanes, alkenes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amines. ***Different ionization and analysis methods: EI, CI, FAB, MALDI, etc.*** Structure determination of molecules.

7. ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY **5 hours**

Principles, presentation of ESR spectrum, DPPH as an external standard, significance of g-values. Hyperfine splitting, hyperfine coupling constants, EPR spectrum of hydrogen atom, isotropic systems involving more than one nucleus (same and different kinds) I = 1/2, 1, 3/2, 5/2 (H, N, Co, Mn, V). Anisotropy in hyperfine coupling, EPR of triplet states, ENDOR and ELDOR techniques.

8. MOSSBAUER SPECTROSCOPY **3 hours**

Principle of analysis, significance of Doppler shift and recoil energy. Procedure for obtaining MS spectra, chemical shift or centre shift/ isomer shift, quadrupole shifting. Magnetic splitting, applications of MS.

REFERENCES

1. Introduction to Spectroscopy, 5th Edition, Donald L. Pavia, Gary M. Lampman, George S. Kriz and James R. Vyvyan, Cengage Learning, 2015.
2. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New-Age International publishers, New Delhi, 2000.
3. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore, 2001.
4. Physical Methods in Inorganic Chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi, 1965.
5. Applications of Absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, 1969.
6. Organic Spectroscopy, W. Kemp, ELBS London, 1975.
7. Infrared Spectra of Inorganic and Co-ordination Compounds, K. Nakamoto, Wiley-Inter-science, New York, 1970.
8. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, 1999.
9. Organic Mass Spectroscopy, K.R. Dass and E.P. James, IBH New Delhi, 1976.
10. Mass Spectrometry of Organic Compounds, H. Budzkiewicz, Djerassi C. and D.H Williams, Holden-Day, New York, 1975.
11. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5th Edition, Saunders College Publishing, London, 1998.
12. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing, New York, 1992.
13. Mass Spectrometry - analytical Chemistry by Open Learning, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, 1987.
14. Modern NMR Techniques for Chemistry Research, Vol. 6, A.E. Derome, Oxford Pergamon Press, 1987.

15. Spectroscopic Methods in Organic Chemistry, 4th Edition, D.H. Williams and I. Fleming, Tata-McGraw Hill Publications, New Delhi, 1988.

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

LO1	Knowledge	Recall the principles, concepts, laws, rules, methods, and sample preparation techniques involved in various spectrometers. Define chromophores, auxochromes, bathochromic shift, hypsochromic shift, hyperchromic shift, hypochromic shift, chemical shifts, integration, spin-spin splitting, and coupling constants in ^{1}H and ^{13}C NMR spectroscopy. Identify vibrational modes associated with different functional groups in IR spectroscopy.
LO2	Understand	Explain hyperfine splitting, coupling constants; g-values in EPR spectroscopy, effects of polar solvents on n-π* and π-π* transitions, impact of conjugation on $\lambda_{max.}$ Elaborate on isotropic and anisotropic systems, zero-field splitting, ENDOR and ELDOR techniques in EPR spectroscopic analysis; stability trends of carbocations and fragmentation patterns in mass spectrometry; principles of 2D NMR, APT, and DEPT techniques in NMR spectroscopic analysis.
LO3	Apply	Identify functional groups using IR spectral data; chemical environment of the nuclei (^{1}H and ^{13}C) using chemical shift values. Determine molecular weights and molecular formulas of organic compounds using *m/z* values in mass spectrometry. Use Woodward-Fischer rules to deduce the spectral shifts of dienes and enones. Compute coupling constants from ^{1}H NMR spectra.
LO4	Analyze	Examine chemical shift, integration, spin-spin splitting, COSY, HETCOR, APT, and DEPT for provided NMR spectra to deduce the structure of organic compounds; relationship between functional groups and their distinctive peaks in an IR spectrum. Investigate the IR, EPR, and Mössbauer spectra to deduce various functional groups, electronic structure, paramagnetic properties (Fe and Sn), and coordination environments of provided compounds.
LO5	Evaluate	Interpret the splitting pattern in the ^{1}H NMR spectrum of a compound. Assess the reliability and limitations of mass spectra, EPR, and Mössbauer techniques in structural determination of organic and inorganic compounds.
LO6	Create	Deduce the molecular structure of unknown compounds using the combined spectral data.

Semester	II
Paper Code	CH 8524
Paper Title	Separation Techniques
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parentheses and italics correspond to recall/review.

1. SOLVENT EXTRACTION **8 hours**

Partition coefficient. Equation for batch extraction and multiple extraction. Extraction efficiency - pH effects. Extraction with metal chelator and crown ethers. Multistage extraction.

2. THEORETICAL ASPECTS OF CHROMATOGRAPHY **6+1 hours**

Types of chromatography. Theoretical principles - retention time, retention volume, adjusted retention time, relative retention, capacity factor. Relation between retention time and partition coefficient. Scaling up, scaling rules. Efficiency of separation, resolution. Ideal chromatographic peaks (Gaussian peak shape). Diffusion, diffusion coefficient. Plate height - Plate height as a measure of column efficiency, number of theoretical plates. Asymmetric peaks. Factors affecting resolution. Band spreading - van Deemter equation, multiple paths, longitudinal diffusion, mass transport. Isotherms and the resulting band shapes. Sample derivatization.

<u>High performance thin layer chromatography, forced flow planar chromatography. 2D TLC. Application of TLC.</u>

3. GAS CHROMATOGRAPHY **(6+2) hours**

Separation process in gas chromatography: schematic diagram - packed column, open tubular columns and comparison with packed columns. Effect of column inner diameter and length of the column. Choice of stationary phase for gas-liquid chromatography and gas-solid chromatography. Retention index, temperature and pressure programming, carrier gas, guard columns and retention gaps. Sample injections - split injection and spitless injection - solvent trapping and cold trapping, on column injection. Detectors: thermal conductivity detector, flame ionization detector, Thermal desorption aerosol gas chromatography (TAG). GC-MS - selected ion monitoring, selected reaction monitoring.

<u>Other Detectors: electron capture detector, nitrogen phosphorous detector, flame photometric detector, photoionization detector, element specific plasma detectors. Sample preparation for GC – head space sampling, solid phase microextraction, purge and trap, thermal desorption. Method development in GC. Applications of GC-MS.</u>

4. LIQUID CHROMATOGRAPHY **(7+2) hours**

Column: stationary phase, bonded stationary phases, monolithic silica columns, elution process - eluent strength, effect of eluent strength of solvent on peak symmetry. Normal phase chromatography, reversed phase chromatography - isocratic and gradient elution. Gradient separations: dwell volume and dwell time, developing a gradient separation. Selecting the separation mode. Injection and detection in HPLC, pumps and injection valves, Method development in HPLC, method development in reversed phase separation. Criteria for adequate separation, optimization with one organic solvent, optimization with two or three different organic solvents, temperature as a variable, choosing a stationary phase. Detectors: spectrophotometric detectors, evaporative light scattering detector. LC-MS, Nano LC-MS: overview, applications in omics.

The chromatographic process - effect of small particles, relation between number of theoretical plates, particle size, column pressure. Solvents- precautions to be taken, Maintaining symmetric band shape. Detectors: characteristics, signal to noise ratio, detection limits, linearity, refractive index detector. Applications of LC-MS.

5. LIQUID CHROMATOGRAPHIC METHODS **(8+1) hours**

Ion Exchange chromatography: Ion exchangers, ion exchange selectivity, selectivity coefficient, Donnan Equilibrium, suppressed ion, anion and cation chromatography, ion chromatography without suppression. Ion pair chromatography. Protein purification using ion-exchange chromatography: isoelectric point (pI) of proteins, effect of pH, buffer selection, choosing the column. Applications.

Size exclusion chromatography: The elution equation, stationary phase, molecular mass determination. Applications. Size exclusion chromatography – Multi angle light scattering (SEC – MALS).

Affinity chromatography: Principle, matrix, ligands, spacer arm - properties required for efficient and effective chromatographic matrix. Immobilized metal affinity chromatography. Other affinity tags: Biotin, GST; post chromatographic removal of affinity tags: TEV protease, thrombin. Applications.

Fast Protein Liquid Chromatography (FPLC) - introduction, FPLC in comparison with HPLC, FPLC columns.

6. CHIRAL CHROMATOGRAPHY – **2 hours**

Principles of chiral chromatography – chiral recognition. Chiral stationary phases (amylose, crown ether, cyclodextrins and pirkle brush type. Applications.

7. SUPERCRITICAL FLUID EXTRACTION AND CHROMATOGRAPHY **2 hours**

Properties of supercritical fluids. Supercritical fluid extraction. Supercritical fluid chromatography: instrumentation and operating variables - effect of pressure, stationary phase and mobile phase. Applications.

REFERENCES
1. Quantitative Chemical Analysis, Daniel C. Harris and Charles A. Lucy, 10^{th} Edn., Macmillan Learning, Austin, 2020.
2. Analytical Chemistry, Gary D. Christian, Purnendu K. Dasgupta and Kevin A. Schug, an Indian adaptation, Wiley, 2020
3. Analytical Chemistry Principles, John H Kennnedy, 2^{nd} Edn, Cengage Delmar Learning India Pvt, 2011.
4. Instrumental Methods of Chemical Analysis, Gurdeep R Chatwal, Sham K Anand, Himalaya Publishing House, 2022.
5. Fundamentals of Analytical Chemistry, D. S Skoog, D. M. West, F. J. Holler, S. R. Crouch, 10^{th} Edition, Cengage Learning, 2022.
6. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 5^{th} edition, Saunders College Publishing, International Limited, 1999.
7. Introduction to modern liquid chromatography, Lioyd R. Snyder, J J Kirkland, J W Dolan, 3^{rd} Edn, Wiley Publication, 2010.
8. Principle and Techniques of Biochemistry and Molecular Biology, Walker Jon and Keith Wilson, 8^{th} Edition, Cambridge University Press, 2018.
9. Sanders KL and Edwards JL. Anal Methods. 2020, 12(36), 4404-4417.
10. Chandarana, C. and Rejji, J., *J Anal Chem,* 78, 2023, 267–293.

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

LO1	Knowledge	Recall the terms, concepts, and theoretical principles of solvent extraction and chromatography
LO2	Understand	Explain/ describe the several factors that affect the efficiency of extraction and separation in solvent extraction and chromatography respectively, ways to improve the same, different types of chromatographic techniques and how to choose the right column for a desired separation
LO3	Apply	Predict ways to improve the extraction of a desired solute taking advantage of the effect of K_D, pH and pKa on extraction and the resolution of a poorly resolved chromatogram Investigate and solve problems associated with peak broadening and poor separation Employ the right chromatographic technique, parameters, stationary and mobile phases for separation of given compounds in a mixture

LO4	Analyze	Compare several methods of purification of a given compound Identify problems/ advantages in each method and finally optimize the best among these methods to obtain a good extraction/ separation
LO5	Evaluate	Justify the choice of solvent and pH used for the extraction of a desired solute Validate the reason for using a particular chromatographic technique, column, flow rate, temperature, stationary and mobile phase for the separation of two compounds/ purification of a protein
LO6	Create	Develop an extraction/ chromatographic method to purify a newly synthesized compound or a newly expressed protein, based on the information obtained from other sources about the properties of the compound/ protein

PRACTICAL PAPERS

Semester	II
Paper Code	CH8P1
Paper Title	PHYSICAL CHEMISTRY PRACTICAL - I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Physical Chemistry Practical-I **(11 sessions)**

1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, energy of activation and Arrhenius parameters for the acid hydrolysis of an ester by volumetry. (1 session)
2. Kinetics of reaction between $K_2S_2O_8$ and KI (salt effect) by volumetry. (1 session)
3. Determination of rate constant for the oxidation of alcohol by colorimetry. (1 session)
4. Determination of partial molal volume of ethanol by reciprocal density method. (1 session)
5. Determination of partial molal volume by apparent molar volume method, NaCl-H_2O system. (1 session)
6. Determination of pK_a of indicators by colorimetry. (1 session)
7. Evaluation of rate constant of first order reaction by potentiometry. (1 session)
8. Colorimetric estimation of aspirin. (1 session)
9. Determination of the Fe by colorimetry. (1 session)
10. Determination of Cu by colorimetry. (1 session)
11. Experiment to be designed by students.

REFERENCES

1. Experiments in Physical Chemistry, Carl Garland, Joseph Nibler, and David Shoemaker and Garland, McGraw Hill International Edition, 2008.
2. Findlay's Practical Physical Chemistry, revised by Levitt, Longman's, London, 1973.
3. Advanced Practical Physical Chemistry, J B Yadav, Krishna Prakashan media, Meerut, India, 2016.

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

LO1	Knowledge	**Define:** i) velocity constant ii) catalytic coefficient iii) temperature coefficient iv) energy of activation v) Arrhenius parameters vi) partial molal volume vii) temperature coefficient for reactions occurring at two different temperatures, activation energy for a reaction. **Recall**: i) the principle behind acid hydrolysis of an ester and the significance of volumetry in this reaction ii) reciprocal density method iii) partial molal volume iv) apparent volume v) the principles of density measurements and their relevance to determining partial molal volume vi) the concepts of partial molal volume of solvent-water system vii) the concepts of partial molar volume of solute-water system viii) the saponification reaction of an ester in the presence of an alkali ix) Arrhenius rate equation for a reaction, units of rate constants. **State** Beer-Lambert law. **Describe**: i) calibration curve ii) the use of spectrophotometer and colorimeter.
LO2	Understand	**Explain**: i) the concept of velocity constant and how it relates to the rate of a chemical reaction ii) the concept of partial molal volume and its significance in understanding solution behavior iii) the principle behind kinetics of reaction acid hydrolysis of ethyl acetate using NaOH, including how reaction rates depend on reactant concentration and temperature, the mechanism involved in the hydrolysis of esters and the role of H^+ ion in catalyzing the reaction iv) the principle involved in the spectrophotometric and colorimetric estimations of analytes **Describe** the role of catalytic coefficient in catalyzed reactions and its impact on reaction kinetics. **Understand**: i) the influence of temperature coefficient on reaction rate and the Arrhenius equation ii) the theory behind the reciprocal density method and how it is used to determine partial molal volume iii) the concept of partial molal volume and apparent molar volume from the experiments of PMV of ethanol-acetone system and salt water systems. **Interpret** the relationship between activation energy and reaction rate.
LO3	Apply	**Apply**: i) the principles of volumetry to determine the velocity constant for the acid hydrolysis of the ester ii) the knowledge of partial molal volume to study the properties of different salt water systems iii) Arrhenius equation to calculate the activation energy of the reaction from the rate constants obtained at different temperatures, temperature coefficient equation to evaluate the rates at two different temperatures. Calculate the catalytic coefficient using experimental data obtained from the reaction. **Utilize**: i) temperature data to calculate the temperature coefficient and Arrhenius parameters ii) the reciprocal density method to calculate the partial molal volume of ethanol. **Prepare** standard solutions in the concentration range of the analyte to plot calibration curve **Plot** calibration curves and calculate the unknown concentration of the analyte. **Operate** the instruments and equipments used in spectrophotometric and colorimetric estimations. **Calibrate** the instruments and equipments used in spectrophotometric and

		colorimetric estimations.
LO4	Analyze	**Analyze**: i) experimental results to identify patterns in the data related to reaction rate and temperature ii) the relationship between density and concentration of ethanol solutions iii) the effect of temperature and concentration of acid on the rate of hydrolysis, comparing the rate constants. **Compare and contrast** the effects of different catalysts on reaction kinetics based on catalytic coefficient values. **Compare** the rate constants obtained from experimental calculation and by graphical plot, the possible experimental errors that can occur leading to deviation from the accurate/expected values. **Optimize** the experimental procedure in terms of sample preparation, reagent quality and instrument errors.
LO5	Create	**Formulate** a hypothesis regarding the effect of varying reaction conditions on the rate of acid hydrolysis of the ester. **Modify**: i) the sample preparation to estimate the analyte from various sources ii) the experiment to estimate the analyte from various sources **Collect** data from various trials and do a statistical data analysis to study accuracy and precision.
LO6	Evaluate	**Critically evaluate** the reliability of experimental data and the accuracy of calculated parameters. **Evaluate** the reliability and accuracy of the kinetic data obtained from the hydrolysis experiment by comparing it with data obtained from other lab student partners. **Compare** different methods of estimation of analytes in terms of time, quality of results and ease of interpretations and reliability of results.

Semester	II
Paper Code	CH8P2
Paper Title	PHYSICAL CHEMISTRY PRACTICAL - II
Number of teaching hours per week	4
Total number of teaching hours per Semester	44
Number of credits	1.5

Physical Chemistry Practical-II **(11 sessions)**

1. Titration of a mixture of strong and weak acids/bases and salt against a strong base/acid by conductometric method. (1 session)
2. Estimation of urea by enzyme hydrolysis using conductance method. (1 session)
3. Determination of dissociation constant of a weak acid or weak base by conductometry. (1 session)
4. Determination of Onsagar parameters for a strong electrolyte by conductometry. (1 session)
5. Determination of thermodynamic parameters of micellization of a surfactant from conductivity measurements. (1 session)
6. Potentiometric estimation of extent of intercalation. (1 session)
7. Titration of a weak acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid. (1 session)
8. Titration of a mixture of strong and weak acids potentiometrically and the determination of the composition of the mixture. (1 session)
9. Determination of activity coefficient of H^+ by potentiometry. (1 session)
10. Degree of hydrolysis of aniline hydrochloride by potentiometry. (1 session)
11. Experiment to be designed by students. (1 session)

REFERENCES

1. Experiments in Physical Chemistry, Carl Garland, Joseph Nibler, and David Shoemaker and Garland, McGraw Hill International Edition, 2008.
2. Findlay's Practical Physical Chemistry, revised by Levitt, Longman's, London, 1973.
3. Advanced Practical Physical Chemistry, J B Yadav, Krishna Prakashan media, Meerut, India, 2016.

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

LO1	Knowledge	**Define**: i) strong acids/bases ii) weak acids/bases iii) salt conductometric method iv) critical micelle concentration v) the dissociation constant and understand its significance in characterizing weak acids or bases vi) micellization and understand its significance in surfactant behavior vii) Onsager parameters and mention their significance viii) intercalation and its significance in materials science and chemistry ix) activity and activity coefficient **Recall**: i) the principles behind the conductometric method and its application in titration ii) the characteristics of strong electrolytes and their behavior in solution iii) the thermodynamic parameters associated with micellization, such as critical micelle concentration (CMC), Gibbs free energy of micellization ($\Delta G°_{mic}$), enthalpy of micellization ($\Delta H°_{mic}$), and entropy of micellization ($\Delta S°_{mic}$) iv) the factors influencing the extent of intercalation in different systems v) the concept of pKa and its significance in acid-base chemistry vi) the principles of potentiometric titration and its application in determining acid compositions vii) critical micellar concentration of surfactants viii) Ostwald's dilution law for a weak electrolyte and the concept of dissociation constant ix) the saponification reaction of an ester in the presence of an alkali x) the definition of pK_a and its significance in acid-base chemistry xi) the definition of the Onsager parameter and its significance in the context of electrolyte solutions xii) the concepts for H^+ ion activity coefficient xiii) the operational principles of a conductometer and potentiometer **Identify** common strong and weak acids/bases and their properties. **State** the significance of urea in biological and clinical contexts. **Explain** i) the principle of enzyme hydrolysis and its role in the breakdown of urea ii) the theory of electrolyte conductivity as described by Onsager's equations. **Describe** the conductance method and its application in quantifying substances based on conductivity changes. **Outline** the principles of potentiometry and its application in studying intercalation processes.
LO2	Understand	**Describe**: i) the difference between strong and weak acids/bases in terms of ionization and conductivity ii) the mechanism of micelle formation and the role of hydrophobic and hydrophilic interactions in stabilizing micelles iii) the principles behind potentiometric titrations

		and how they are utilized to determine pKa values **Explain**: i) how the conductometric method measures the progress of a titration ii) the enzymatic reaction involved in the hydrolysis of urea by the urease enzyme iii) the mechanism of intercalation and its impact on the electrochemical properties of materials iv) the principle of quinhydrone electrode and its application in potentiometric titrations v) Nernst equation vi) role of water and the formation of products such as aniline and hydrochloric acid vii) the concept of conductivity and how it relates to the concentration of ions in a solution. **Discuss**: i) the relationship between the concentration of urea and the conductivity of the solution in the context of the conductance method ii) the relationship between the degree of ionization of a weak acid or base and its dissociation constant iii) the factors influencing micellization, including surfactant concentration, temperature, and solvent properties iv) the concept of titration curves and how they vary for different acid-base combinations. **Interpret**: i) the mechanism behind how the conductance method measures urea concentration ii) the theoretical background behind determining Onsager parameters from experimental conductance data iii) the significance of pK_a values in characterizing weak acids and their ionization behavior iv) the titration curve obtained from potentiometric titration of acid mixtures v) experimental data obtained from potentiometric measurements and applying this knowledge to determine the degree of hydrolysis. **Understand** i) the relationship between ion mobility, concentration, and conductivity in strong electrolytes as described by Onsager's equations ii) the concept of potentiometric titration and how it measures the change in electrode potential during acid-base reactions, the concept of activity iii) how they relate the activity of H^+ ions in solution iv) difference between different types of electrodes used in potentiometer such as standard hydrogen electrode (SHE) and saturated calomel electrode v) the importance of conductometry to determine the K_a of a weak acid vi) the kinetics of saponification using conductance measurements vii) the accurate methods to prepare solutions, standardizing the primary and secondary standard solutions viii) the differences between working electrode and reference electrode and using quinhydrone electrode in potentiometer experiments

		Outline the concept of conductometric measurements and how they relate to the Onsager parameters. **Comprehend:** the chemical reaction involved in the hydrolysis of aniline hydrochloride
LO3	Application	**Perform** i) a titration of a mixture of strong and weak acids/bases and salt against a strong base/acid using the conductometric method ii) the urea estimation experiment using the enzyme hydrolysis method coupled with conductance measurements. **Determine** the equivalence point of the titration based on conductometric data. **Apply** i) appropriate calibration techniques to relate conductance readings to urea concentrations ii) mathematical techniques to analyze the conductance data and calculate the dissociation constant iii) mathematical techniques to analyze the conductance data and calculate the Onsager parameters iv) appropriate calibration techniques to relate potential changes to the progress of the titration v) theoretical concepts from electrochemistry and chemical kinetics to understand the factors vi) the conductometric method to determine K_a of a weak acid and verify Ostwald's dilution law, the conductometric measurements to determine Arrhenius parameters such as pre-exponential A, activation energy and rate constant vii) potentiometric titrations to obtain strengths of acid mixture viii) conductometric titrations to obtain strengths of base mixture **Use** i) a conductometer to determine the dissociation constant of a weak acid or weak base ii) a conductometer to determine the Onsager parameters for a strong electrolyte iii) a conductometer to determine the thermodynamic parameters of micellization for a surfactant iv) potentiometric measurements to estimate the extent of intercalation v) a quinhydrone electrode and perform the titration of a weak acid against a strong base vi) a potentiometer to carry out a titration of a mixture of strong and weak acids. Calculate activity coefficient of H+ ions using emf of the cell . **Utilize**: i) the data obtained from the potentiometric titration to calculate the pKa values of the dibasic acid ii) the experimental data obtained from the conductometric measurements to calculate the Onsager parameter.
LO4	Analysis	**Analyze**: i) the conductometric data obtained during the titration to determine the concentrations of the acids/bases in the mixture ii) the

		conductance data obtained during the experiment to determine the concentration of urea in the sample iii) the conductance data obtained and relate it to the strength of the acid or base iv) the experimental conductance data to determine the limiting equivalent conductivity and association constant of the strong electrolyte v) the experimental conductance data to determine the critical micelle concentration (CMC) and other thermodynamic parameters of micellization vi) the potentiometric data obtained during the experiment to estimate the extent of intercalation vii) quantitatively determine the degree of hydrolysis of aniline hydrochloride using potentiometric measurements viii) the experimentally obtained value of K_a and compare them with the graphical results ix) the titration curve obtained from the potentiometric titration to identify equivalence points and half-equivalence points x) the titration on a graph and obtain the strengths of the acids/bases in an acid mixture or a base mixture . **Interpret**: i) the shape of the conductometric titration curve and relate it to the nature of the acids/bases being titrated ii) trends in conductance readings and relate them to changes in urea concentration iii) the conductance curves to extract information about the nature of the electrolyte iv) the behavior of the surfactant solution near the CMC and relate it to micelle formation v) the titration curve to calculate the pKa value of the weak acid vi) the titration curve to calculate the composition of the acid mixture, including the concentrations of strong and weak acids. **Compare and contrast** the behavior of different electrolyte solutions based on their Onsager parameters.
LO5	Create/Synthesis	**Design and execute**: i) variations of the titration experiment to investigate different acid/base mixtures and concentrations ii) variations of the experiment to explore factors influencing the accuracy and precision of urea estimation by enzyme hydrolysis using the conductance method. **Formulate** hypotheses about the behavior of acids/bases in various titration scenarios and design experiments to test these hypotheses. **Design:** i) experiments to investigate the effect of varying experimental parameters (such as concentration, temperature, or pH) on the determination of dissociation constant ii) experiments to investigate the effects of varying parameters such as concentration, temperature, and solvent on the determination of Onsager parameters iii) experiments to

		investigate the effects of varying parameters such as temperature, surfactant structure, and solvent composition on the thermodynamic parameters of micellization. **Develop** protocols for accurately determining Onsager parameters for different strong electrolytes using conductometric methods.
LO6	Evaluate	**Compare and contrast** the advantages and limitations of conductometric titration compared to other titration methods. **Reflect** i) on the practical applications of conductometric titration in real-world analytical chemistry contexts ii) on the practical applications of urea estimation in fields such as clinical diagnostics, environmental monitoring, and food analysis iii) on the practical implications of understanding dissociation constants in fields such as chemistry, biochemistry, and pharmaceuticals iv) on the practical implications of understanding Onsager parameters in fields such as physical chemistry, electrochemistry, and materials science v) on the practical implications of understanding intercalation processes in fields such as battery technology, catalysis, and materials science vi) on the practical implications of understanding pK_a values in fields such as pharmaceuticals, biochemistry, and environmental chemistry **Compare** i) the conductance method for urea estimation with other analytical techniques, considering factors such as sensitivity, specificity, and ease of implementation ii) the advantages and limitations of conductometry for determining dissociation constants with other methods iii) the advantages and limitations of using conductometric methods for determining thermodynamic parameters of micellization with other techniques iv) the advantages and limitations of using quinhydrone electrode titrations to determine pK_a values with other techniques v) the advantages and limitations of using potentiometric titration for determining acid mixture compositions with other analytical techniques. **Evaluate** strength of unknown solutions containing two different acids or bases

Semester	II
Paper Code	CH 8P3
Paper Title	SYNTHESIS AND CHARACTERIZATION OF COMPOUNDS- I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

List of experiments **(11 sessions)**

1. Preparation and quantitative analysis of hexamminecobalt (III) chloride. (2 sessions)
2. Preparation of potassium trioxalatoferrate(III) trihydrate and its characterization by quantitative analysis and IR studies. (2 sessions)
3. Preparation of a variety of complexes and their characterization by UV-Visible and IR techniques. (2 sessions)
4. Preparation of a nano material/metal-organic framework and its characterization by UV spectroscopy (band gap) and XRD (crystallite size). (2 sessions)
5. Synthesis of spinel and its characterization by XRD studies. (2 sessions)
6. Any other experiment/viva (1 session)

REFERENCES

1. Experimental Inorganic/Physical Chemistry, M. A. Malati, Woodhead Publishing Limited, 1999.
2. Vogel's Textbook of quantitative chemical analysis; J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, 6th edition, Pearson Education Limited, 2009.
3. Integrated Approach to Coordination Chemistry, R. A. Marusak, K. Doan, S. D. Cummings, John Wiley & Sons, 2007.
4. Advanced Practical Chemistry, 2^{nd} Ed., J. Singh, L. D. S. Yadav, R. K. P. Singh, I, R. Siddiqui, J. Singh, J. Srivastava, Pragati Prakashan, 2010.
5. Practical Inorganic Chemistry, G. Pass, H. Sutcliffe, Chapman and Hill, 1974.
6. Electronic Absorption Spectroscopy and Related Techniques, D. N. Sathyanarayana, Universities Press, 2001.
7. Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A, B: 6^{th} Ed., K. Nakamoto, John Wiley & Sons, 2009.

Learning outcomes: After learning this course, the student should be able to:

LO1	Knowledge	Outline the method of preparation of square planar and octahedral complexes Write the protocol for the preparation of different coordination complexes/inorganic materials Record the details of the preparation of coordination complexes/inorganic materials and their spectral/volumetric analyses
LO2	Understand	Explain various factors that determine the formation of

		complexes/inorganic materials
LO3	Apply	Modify the reaction conditions for the preparation of various complexes/inorganic materials for comparative study Estimate of the constituents of complexes/inorganic materials based on the principles of volumetric analyses Compare the theoretical and experimental weight percentages of constituents of a complex
LO4	Analyze	Interpret the spectroscopic/XRD/TGA data of prepared complexes/inorganic materials, nature of bonding and types of transitions giving spectral bands Compare the UV/IR spectral data of *cis* and *trans* isomers
LO5	Evaluate	Predict the structure/properties of complexes/inorganic materials by IR/UV, TGA, DTA, XRD
LO6	Create	Develop new protocols/methods for the preparation of metal complexes of low (2-5) and high coordination numbers (7-10), geometrical isomers: tetrahedral, square planar, cis- trans, facial, meridional isomers of octahedral complexes

Semester	II
Paper code	CH8P4
Paper title	SYNTHESIS AND CHARACTERIZATION OF COMPOUNDS-II
Number of teaching hours per week	4
Total number of teaching hours persemester	44
Number of credits	1.5

Organic Synthesis, purification and characterization **(11 sessions)**

1. Synthesis of benzanilide from benzophenone (2 sessions)

2. Synthesis of benzilic acid from benzoin (2 sessions)

3. Synthesis of anthranilic acid from phthalic acid (2 sessions)

4. Synthesis of 2-iodoxy benzoic acid (IBX) from anthranilic acid and its application for the oxidation of alcohol (3 sessions)

5. Synthesis of dibenzalacetone and reduction of carbonyl group (2 sessions)

6. Application of *N*-bromosuccinimide (NBS) in allylic bromination (1 session)

7. Synthesis of an organic compound (one step preparation) by 2 or 3 different methods and comparison/evaluation of the methods with respect to the following parameters

(1-2 sessions)

(i) Ease of preparation, problems in handling chemicals, toxicity and flammability of chemicals

(ii) Yield and cost effectiveness

(iii) Product purity/quality

(iv) Environmental compatibility (from the point of view of green chemistry).

8. Any other related experiments/ RBPT

Characterization of the organic compounds by: TLC, column liquid chromatography, UV and IR spectroscopic techniques.

REFERENCES

1. Handbook of Preparative Inorganic Chemistry, G Brauer, Academic Press, 1963.
2. Practical Inorganic Chemistry, Marr and Rocket, 1972.

3. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari, 1996.
4. Practical Organic Chemistry, Mann and Saunders, 1980.
5. Textbook of Practical Organic Chemistry, A I Vogel, 1996.
6. A Handbook of Organic Analysis, Clarke and Hayes, 1964.

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

LO1	Knowledge	Recall various oxidation, reduction and substitution reactions, safety protocols and procedures for handling organic chemicals and equipment. Write suitable chemical reactions for the planned synthesis
LO2	Understand	Write the mechanisms of various organic reactions Visualize reaction set up under reflux, inert and other suitable conditions
LO3	Apply	Apply various oxidizing, reducing and other reagents to synthesise target organic molecule; spectroscopic methods (e.g., NMR, IR) to identify and confirm the homogeneity of the prepared organic compound
LO4	Analyse	Analyse the results of organic reactions to determine the efficiency of the synthesis and the purity of the products Examine the reasons for failure of the reaction, low yield or formation of byproducts Demonstrate the green chemistry aspects of the reaction
LO5	Evaluate	Evaluate experimental designs and propose improvements to optimize reaction conditions and to increase yields maintaining appropriate safety measures and assess green chemistry aspects
LO6	Create	Design alternate routes for the preparation of specific target molecules

Semester	III
Paper code	CH9125
Paper title	BIOLOGICAL CHEMISTRY
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study**.**
2. Text within parentheses and italics correspond to recall/review.

1. ESSENTIAL AND TRACE ELEMENTS IN BIOLOGICAL SYSTEMS (2 + 1) hours

Role of metal ions in biological processes. Metal ion toxicity and detoxification - chelation therapy. Metal complexes in medicine: gold complexes and platinum complexes.

2. METAL ION STORAGE AND TRANSPORT (4+2) hours

Ferritin, transferrin, ceruloplasmin, siderophores. ***Transport and storage of dioxygen: hemoglobin, myoglobin; phenomenon of cooperativity;*** model systems (picket fence porphyrins), hemocyanin and hemerythrin.

3. TRANSPORT OF IONS ACROSS MEMBRANES 6 hours

Active and passive transport across the membrane, ion transport, crown ether and cryptands. Naturally occurring antibiotics: valinomycin, nonactin, gramicidin. Mechanism of ion transport: sodium potassium pump and Na^+/K^+ ATPase. Chemistry of vision and nerve conduction.

4. ELECTRON TRANSPORT PROTEINS 6 hours

Rubredoxin, ferredoxins, cytochromes. Photosynthesis: chlorophyll, PS I, PS II, role of manganese-protein complex in electron transfer in photosynthesis. Nitrogen fixation: bacterial nitrogenase system. Biochemical importance of NO. Role of Ca in signal transduction.

5. ENZYMES 7 hours

Mechanism of enzyme action. Examples of some typical enzyme mechanisms - chymotrypsin, lysozyme. Michaelis-Menten kinetics and derivation of the equation, modifications and extensions of Michaelis-Menten equation, significance of Michaelis-Menten parameters, graphical representation of data - Lineweaver-Burke and Eddie Hoftsee plotlots, enzyme inhibition kinetics (competitive, non-competetive, uncompetitive and mixed). Non-productive binding. Competing substrates. Reversibility – Haldane equation. Breakdown of Michaelis-Menten equation. Multisubstrate systems – brief description of different mechanisms (ordered, sequential and random).

6. METALLOENZYMES **9 hours**

Non-redox enzymes – carboxypeptidase A and carbonic anhydrase; redox enzymes - superoxide dismutase (mono and binuclear), peroxidase, catalase, cytochrome oxidase, Cyt P_{450}, ascorbic acid oxidase, alcohol dehydrogenase; cobalamine (coordination environment around the metal and mechanism of action of each enzyme to be discussed).

7. COENZYMES **7 hours**

Structure and typical reactions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid (one representative mechanism for each type of reaction).

8. BIOSYNTHESIS OF MACROMOLECULES **7 hours**

Pseudocycles - gluconeogenic pathway and its regulation. Biosynthesis of cholesterol and its regulation. Protein synthesis: genetic code, wobble hypothesis, five stages of translation – i) activation (including idea of regulation of aminoacyl t-RNA synthesis) ii) initiation process (including significance of Shine-Delgarno sequence) iii) elongation iv) termination and v) posttranslational modification.

9. BIOENERGETICS **(3 + 2) hours**

Standard free energy change in biochemical reactions. Ways in which non-spontaneous reactions are overcome. ATP hydrolysis and synthesis, energy generation in mechano-chemical systems: muscle contraction.

10. BIOPOLYMER INTERACTIONS **(2+2) hours**

Electrostatic charges, hydrophobic forces, dispersion forces. Various types of binding processes in biological systems.

REFERENCES:

1. Principles of Biochemistry, David L.Nelson and Michael M.Cox 8th Edn., Macmillan Learning, 2021.
2. Biochemistry, L. Stryer, 10th Edn., Macmillan Learning, 2023.
3. Principles of Biochemistry, G. Zubay 4th Edn., Mcgraw Hill, 1998.
4. Biochemistry, Voet and Voet, 5th Edn., John Wiley 2018.
5. Organic Chemistry, Paula Bruice, 8th Edn., Pearson, 2020.
6. Bioinorganic chemistry, Asim K. Das, Books and Allied publishers (P) Ltd., Kolkata, 2015.

7. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, Viva Books Pvt. Ltd., 1998.
8. Enzymes: Structure and Function, S Blackburn Marcel Dekker, 5th Edn., 2000.
9. Physical Chemistry with Applications to Biological Systems, Raymond Chang, McMillan, 1977.
10. Bioorganic and Supramolecular Chemistry, P.S. Kalsi , J. P. Kalsi , and Ashu Chaudhary, New Age International publishers, 2020.

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

LO1	Knowledge	Define various types of catalytic mechanisms and biopolymer interactions, coupling of reactions, non-productive binding and competing substrates Identify the type of reversible inhibitions based on k_m and V_{max} values Write balanced chemical reactions for ATP synthesis, emphasizing even the reverse process of ATP hydrolysis Describe role of different metal ions in biological system including coordination chemistry, redox reactions
LO2	Understand	Differentiate between sequential and ping-pong mechanisms in multi-substrate reactions, explain the order in which substrates bind and products are released Explain the mechanisms of chymotrypsin and lysozyme, the energy input required for ATP synthesis, such as the proton motive force in oxidative phosphorylation, the structures of metalloproteins, the mechanism of transportation and release of elements like O, Fe in biological system Describe the importance of translation and post-translational modifications in the maturation and functionality of proteins. Interpret the Michaelis-Menten plot, illustrating the relationship between substrate concentration and initial reaction velocity. Discuss the various regulatory mechanisms that control the biosynthesis of macromolecules Recognize the applications of the fundamental principles of inorganic chemistry to bioinorganic systems Identify the role of trace elements in life’s processes
LO3	Apply	Relate ATP hydrolysis to specific cellular processes, including muscle contraction, active transport, and biosynthetic reactions, catalytic efficiency to enzyme effectiveness Compare and contrast the various types of reversible inhibitions. Solve and apply the Michaelis-Menten equation/ Lineweaver Burke

		equations and plots to explain enzyme behavior Apply knowledge of bioinorganic chemistry principles to analyze and solve complex problems related to metal ion, Modify the existing metal-based drugs for better selectivity
LO4	Analyze	Calculate the catalytic efficiency and turnover numbers in single substrate reactions, and relate them to the enzyme's efficiency Illustrate the mechanism and role of coenzymes in catalyzing diverse biochemical reactions, such as carriers of electrons and functional groups Examine the redox property of metal ions in biological systems. Compare the efficacy of different types of metals in biomedical application
LO5	Evaluate	Assess the experimental data and scientific literature to judge the contribution of bioinorganic chemistry to our understanding of biochemical phenomena, and to identify emerging trends and unanswered questions in the field Evaluate the efficiency of biocatalyst at different temperature and pH.
LO6	Create	Propose suitable mechanism of action for enzymes Design and propose innovative approaches for studying and manipulating metal-ion mediated biological processes Integrate concepts of bioinorganic chemistry with techniques from other scientific disciplines to address complex biological challenges

Semester	III
Paper Code	CH9225
Paper Title	ORGANOMETALLIC CHEMISTRY AND INORGANIC REACTION MECHANISMS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.
2. Text within parentheses and italics correspond to recall/review.

1. ORGANOMETALLIC COMPOUNDS **(5+2) hours**

Nomenclature of organometallic compounds; ***classification based on the hapticity of ligands and the polarity of C-M bond***; 18- electron rule, electron counting - covalent and ionic models; thermal, thermodynamic and kinetic stability and decomposition pathways; ***general methods of synthesis of organometallics of representative elements.***

2. ORGANOMETALLIC COMPOUNDS OF MAIN GROUP ELEMENTS **7 hours**

Group trends; structure and bonding in Li, Be, Mg and Al alkyls.

3. ORGANOMETALLIC COMPOUNDS OF TRANSITION METALS **(11+3) hours**

Classification, structure, bonding, ***general methods of preparation and important classes of reactions of transition metal alkyls***, carbenes and carbynes; structure and bonding in transition metal complexes with dihapto to octahapto-donor ligands - alkene, allyl, 1,3-butadiene, cyclopentadienyl, ***arene, cycloheptatrienyl and cyclooctatetraenyl complexes***; metallocenes with special reference to ferrocene, cyclometallation and ring slippage reactions; ***activation of small molecules (CO and alkanes)***; isolobal analogy and its applications.

4. ORGANOMETALLIC COMPOUNDS IN ORGANIC SYNTHESIS **(14+2) hours**

Green's rules; use of iron and chromium carbonyls in the synthesis of aromatic compounds; rhodium complexes in hydrogenation, hydroformylation, decarbonylation reactions; Monsanto acetic acid process; ***palladium complexes in the synthesis of carbonyl compounds***; Heck reaction; Wacker process; applications of zinc dialkyls, Grignard reagents, lithium alkyls, Gilman reagents (lithium dialkyl cuprates); ***organocadmium,*** organoselenium, organoaluminium, ***organosilicon, organotin and organomercurials in organic synthesis***. Zeigler-Natta catalysts (growth reaction, polymerization of olefins).

5. INORGANIC REACTION MECHANISMS (15+1) hours

Kinetic lability and inertness, classification of metal ions based on lability; types of nucleophilic substitution reactions; kinetics and mechanism of nucleophilic substitution in square planar and octahedral complexes - trans effect; ligand field effects and reaction rates; reaction rates influenced by acids and bases, SN1CB mechanism; racemization and isomerization; mechanisms of redox reactions - outer sphere mechanism, Marcus equation for outer sphere cross reactions, excited state outer sphere electron transfer reactions, photochemical reactions of ruthenium complexes, inner sphere mechanism; oxidative addition and reductive elimination; migratory insertion; ***nucleophilic and electrophilic attack on coordinated ligands***; template reactions.

REFERENCES

1. Organometallic Chemistry, R. C. Mehrotra and A. Singh, Wiley Eastern (1991).
2. The Organometallic Chemistry of the Transition Metals, R. H. Crabtree, 6th edition, John Wiley & sons (2014).
3. Organometallics, Vol 1 & 2, M. Bochmann, Oxford Chemistry Primers, Oxford University Press (1994).
4. Organometallic Reagents in Synthesis, Paul R. Jerkins, Oxford Chemistry Primers, Oxford University Press (1992).
5. Principles of Organic Synthesis, Sir Richard Norman and James M Coxon, 3rd edition, Chapman & Hall (1993).
6. Modern Synthetic Reactions, H. O. House and Benjamin (1972).
7. Reaction Mechanisms of Inorganic and Organometallic Systems, J. B. Jordan, Oxford University Press, 2nd edition (1998).
8. Inorganic Chemistry, G. L. Miessler, P. J. Fischer and D. A. Tarr, 5th edition, Pearson Education (2014).
9. Inorganic Chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th edition, Addison-Wesley (1993).
10. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B. D. Gupta and Anil J. Elias, 2nd edition, universities press (2013).

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

LO1	Knowledge	Recall IUPAC nomenclature, classification, applications of organometallic compounds, hapticity of ligands, group trends exhibited by main group organometallics, kinetic lability and inertness
LO2	Understand	Discuss general methods of preparation/bonding in transition metal

		alkyls, carbenes, carbynes, transition metal complexes with dihapto to octahapto pi-donor ligands/ferrocene/ main group organometallic compounds, types and factors affecting nucleophilic substitution reactions in coordination complexes; reactions/mechanisms/catalytic cycles involving organometallic compounds, cyclometallation, and ring slippage reactions, the applications of carbonyls, rhodium complexes, Pd complexes, zinc dialkyls, Grignard reagents, organo-Cd/Se/Al/Si/Sn/Hg in organic synthesis Describe the kinetics and mechanisms of nucleophilic substitution in square planar and octahedral complexes Differentiate the bonding between carbene and carbyne transition metal complexes, the mechanisms of inner-sphere and outer-sphere reactions Explain the classification of organometallic compounds based on the hapticity of ligands and bond polarity; thermodynamic and kinetic stability and decomposition pathways of organometallic compounds, activation of small molecules; β-hydride elimination in transition metal-alkyl complexes
LO3	Apply	Illustrate the bonding in Zeise's salt, ferrocene, racemization and isomerization in optically active octahedral complexes Derive the rates of reactions of nucleophilic substitution in metal complexes Predict the bond properties of organometallic compounds by using isolobal analogy, the position of attack on polyenes/enyls based on Green's rules, the products of reaction catalyzed by organometallic compounds, the structural similarities and differences among alkyl compounds of Li, Be, Mg, and Al. Compute the valence electron count based on 18 e^- rule.
LO4	Analyze	Identify the ring slippage reactions for given complexes, outer-sphere reaction mechanism for photo-catalytic Ru-complexes
LO5	Evaluate	Predict the structure and bonding for given transition metal complexes, electron transfer reactions in metal complexes Assess the effectiveness of different organometallic compounds in specific synthetic applications
LO6	Create	Outline the outer-sphere and inner-sphere mechanism for various redox reactions Design the synthetic routes for target organic molecules with specific properties utilizing organometallic compounds

Semester	III
Paper code	CH9325
Paper title	ELECTROCHEMISTRY AND ELECTROANALYTICAL TECHNIQUES
Number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

NOTE: 1. Text underlined, bold and in italics correspond to self-study.
2. Text within parentheses and italics correspond to recall/review.

1. THEORY OF STRONG ELECTROLYTES 8 hours

Ionic atmosphere, Debye-Hückel theory of ion-ion interaction, Debye-Hückel equation in terms of activity coefficient, Debye-Hückel limiting law. Debye-Hückel equation for appreciable concentration, Hückel and Brønsted equation. Qualitative verification of the Debye-Hückel equation, ion association - ion pairs and triple ions and conductance minima.

2. ELECTRIFIED INTERFACE AND ELECTRODICS (10 + 2) hours

The electrified interface: surface excess, interfacial tension and its determination, electrocapillary curves, thermodynamics of electrified interface — Lippmann equation, determination of the electrical capacitance of the interface, determination of surface excess. Structure of electrical double layer — Helmholtz-Perrin model, Gouy-Chapman diffuse charge model and Stern model. Electrodics: electron transfer under an interfacial electric field, equilibrium and exchange current densities, overpotential — dependence of current density on overpotential. Butler-Volmer equation and its special cases, the symmetry factor, influence of current density, pH and temperature on overvoltage. Tafel equation-derivation, Tafel plot.

<u>Theories of overvoltage. Bubble formation as the slow process, combination of atoms as the slow process, ion discharge as the slow process and proton transfer as the slow process.</u>

3. ELECTROANALYTICAL TECHNIQUES 25 hours

a. ELECTROPHORESIS AND ELECTROCHROMATOGRAPHY (3+1) h

Important terms in electrophoresis, basis of electrophoretic separation. Expression for distance traveled on application of electrode potential. Role of buffer in electrophoresis.

Classical gel electrophoresis, high performance capillary electrophoresis – advantages. Instrumentation, sample injection. Comparison of classical and capillary electrophoresis.

Electroosmotic flow. Modes of electrophoresis: capillary gel electrophoresis, capillary isoelectric focusing, and capillary isotachophoresis.

Capillary electrochromatography (basic principle). Micellar electrokinetic capillary electrophoresis.

b. ION SELECTIVE ELECTRODES (4+ 1) h

Potentiometry: electrodes used - metallic indicator electrodes (types with one example for each), metallic redox indicator electrodes, ion selective electrodes (ISE) - classification of ISE. Properties of ISE.

Glass membrane electrodes. Composition and structure of glass membrane. Hygroscopicity of glass membrane. Electrical conductance across the glass membrane. Membrane and boundary potential. Expression for E_b. Alkaline error. Crystalline membrane electrodes. Conductance of a crystalline membrane electrode.

Fluoride electrode. Electrodes based on silver salts. Liquid membrane electrode for Ca^{2+}. Molecular selective electrode systems. Gas sensing probe for CO_2.

Two types of gas sensing membrane materials, Biocatalytic membrane electrodes (two types of electrodes for the determination of BUN).

c. VOLTAMMETRIC TECHNIQUES (14+2) h

Polarization: ideal polarized and ideal non-polarized electrodes - sources of polarization. Reaction and concentration polarization. Mechanism of mass transport. The current response to applied potential (in terms of Fermi level and molecular orbitals) Faradaic and non-Faradaic currents. Charging and residual currents.

Polarography: Advantages of Hg over other solid electrodes. Types of mercury electrodes: DME, SMDE, HMDE and MFE. Instrumentation, potentiostat, function generator, three electrode system, and supporting electrolyte. Polarographic/IUPAC convention. Polarographic experiment. Polarographic parameters (diffusion current, half wave potential and their significance). Analysis of a polarogram. Effect of dissolved oxygen on electrochemical reduction process. Ilkovic equation (derivation). Quantitative and qualitative aspects of voltammetry: determination of concentration and standard state potentials. Determination of electrochemical reversibility and number of electrons. Effect of complex formation on polarographic waves. Determination of metal-ligand stoichiometry.

Potential excitation and response signal, and the corresponding voltammetric techniques: Linear scan polarography / voltammetry (LSP/V), staircase voltammetry (SV), normal pulse

(NPP/V), differential pulse (DPP/V), square wave (SWV) and cyclic voltammetry. Applications of polarography. Amperometric titrations at DME (all four types). Stripping voltammetry: cathodic, anodic and adsorption stripping voltammetry.

Cyclic voltammetry: excitation signal and current response in CV. Important parameters of CV. Instrumentation. Reversible, irreversible and quasireversible charge transfer and the diagnostic criteria. A cyclic voltammetric experiment - analysis of a cyclic voltammogram of potassium ferricyanide system. Cathodic and anodic processes. Working electrodes in voltammetry (glassy carbon, carbon paste, gold, platinum and modified electrodes). Coupled chemical reactions.
Coulometric methods of analysis: controlled-potential and controlled-current coulometry. Coulometric titrations, quantitative applications. Chronoamperometry and chronopotentiometry.

REFERENCES:

1. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science; Amulya K.N. Reddy O'M. Bockris; 2nd edition, Kluwer Academic, New York (2010).
2. An Introduction to Electrochemistry by Samuel Glasstone, Read Books Ltd, (2013), (e- book).
3. Principles of Instrumental Methods of Analysis, Skoog, Holler and Nieman, 7th edition, CENGAGE Learning, Boston, USA (2016).
4. Analytical Chemistry Principles – John H Kennedy, 2nd edition, Cengage India (2011).
5. Modern Analytical Chemistry David Harvey; 1st edition, McGraw-Hill Higher Education, USA (2000).
6. Vogel's Textbook of Quantitative Chemical Analysis, 6th edition, Pearson Education Limited (2007).
7. Electrochemical Methods – Fundamentals and Applications, Allen J Bard and Larry R. Faulkner, 2nd edition, John Wiley and Sons, USA (2001).

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

LO1	Knowledge	**Recall**: The concept of the ionic atmosphere and its significance in solution behavior, fundamental principles of the Debye-Hückel theory of ion-ion interactions, the Debye-Hückel equation, and its terms. **Identify**: Factors influencing the activity coefficient in the Debye-Hückel equation, components of the Lippmann equation and its application in determining interfacial properties, models used to describe the structure of the electrical double layer. **Outline**: Key components of electrodics, including electron transfer

		processes and overpotential, role of buffers in electrophoresis and their importance in maintaining pH stability and charge neutrality. **Define**: Electrophoretic mobility and its relation to the charge of the solute, migration, migration velocity, Zeta potential, electroosmotic force, and running buffer, potential window, Faradaic and non-Faradaic currents, residual currents. **List**: Examples of metallic indicator electrodes and metallic redox indicator electrodes, classifications of ion-selective electrodes (ISE) and properties associated with ISE. **Describe**: Debye-Hückel limiting law, polarization in electrochemical systems and sources of polarization, concepts of charging and residual currents in polarography, advantages of mercury electrodes over other solid electrodes, different voltammetric techniques and their applications. **Discuss**: Diagnostic criteria for electrochemical reversible, quasi-reversible, and irreversible processes.
LO2	Understand	**Explain**: The Debye-Hückel limiting law and its implications for dilute solutions, physical meaning and mathematical representation of the Debye-Hückel equation, modification of the Debye-Hückel equation for appreciable concentrations, ion association, ion pairs, and triple ions, and their role in solution conductance, principles behind determining electrical capacitance and surface excess at the electrified interface, Helmholtz-Perrin, Gouy-Chapman, and Stern models of the electrical double layer and their implications, equilibrium concepts, exchange current densities, and their dependence on overpotential and anisotropic nature of forces at the interface and exchange current density. **Interpret and Comprehend**: Electrocapillary curves and their relationship to interfacial properties and electric fields, distance traveled by particles in electrophoresis with respect to electrode potential, its relation to particle charge and size, basic principles underlying electrophoretic separation, factors influencing particle distance under an applied electrode potential, the differences between classical gel electrophoresis and high-performance capillary electrophoresis, their advantages and limitations. **Describe and Discuss**: Capillary isotachophoresis technique and the order of separation of species, reversal of electroosmotic flow, capillary electrochromatography, instrumentation required for

		classical and capillary electrophoresis, the sample injection process, mobilization of focused bands using capillary isoelectrofocusing technique, separation of cations by various electrophoretic methods, and order of elution in electrochromatography and MEKC capillary method of separation. **Discuss**: Instrumentation and sample injection methods for electrophoretic experiments, construction of an electrochemical cell with a glass electrode coupled with a calomel electrode for measuring unknown pH, properties, and applications of ion-selective electrodes and metallic electrodes, the construction of LaF_3, liquid membrane electrodes and the mechanism of potential development, a gas-sensing probe for determining CO_2, hygroscopy of glass membrane electrode, its composition, its structure, and electrical conductance across the glass membranes, boundary potential in potentiometry, alkaline error, biocatalytic membrane electrodes, and their applications, the current response to an applied potential using Fermi levels and frontier orbitals, different modes of mass transport in voltammetry, principles of polarography, voltammetry, reversible, irreversible, quasi-reversible charge transfer in cyclic voltammetry. **Differentiate**: Faradaic vs. non-Faradaic currents, capillary and classical electrophoresis, residual and non-residual currents, DPV and NPV. **Discuss and Interpret**: Amperometric titration for determining equivalence points, interpretation of cyclic voltammograms, working principles of different electrodes in voltammetry and coupled chemical reactions in voltammetric analysis.
LO3	Apply	**Apply**: the Debye-Hückel equation to calculate activity coefficients, the Hückel and Brønsted equations to predict behavior of electrolyte solutions, the Butler-Volmer equation and Tafel equations to analyze electrodics, relevant theory to predict the shielding effect of electrolytes, thermodynamics to derive the Lipmann equation, Exchange current density values to calculate current density, Lipmann equation. **Derive**: the Debye-Hückel equation for solutions of appreciable concentration, the Debye-Hückel-Brønsted equation to account for the polarisation of solvent molecules, the potential of an electrolyte using Debye-Hückel theory, the hyperbolic sine wave function when

		$\alpha = 0.5$, equilibrium constants of coupled chemical reactions using the polarographic technique, maximum current using Ilkovic's theory, and metal-ligand stoichiometry using polarography. **Predict** the mean ionic activity coefficient using the given data. **Use**: the Butler-Volmer equation to derive the Tafel equation, electrophoresis principles to predict migration behavior under different conditions. **Illustrate and Predict**: Reversal of electroosmotic flow in capillary electrophoresis, elution order in separation methods like MEKC and capillary isotachophoresis, location of neutral molecules in capillary electrophoresis, elution order in separation of low molecular weight nitro compounds using the MEKC method. **Apply and Determine**: molecular selective electrode systems and gas sensing probes in specific scenarios, Nernst equation and extract qualitative aspects from voltammograms, formation constants and stoichiometry of complexes. **Apply and Utilize**: Amperometric titration technique for determining unknown concentration of the analyte, voltammetric techniques for specific analytical purposes, including quantification and identification, diagnostic criteria to identify reversible, quasi-reversible, and irreversible processes.
LO4	Analyze	**Analyze and Compare**: Experimental data to determine the validity of the Debye-Hückel equation for different electrolyte solutions, the behavior of electrolyte solutions based on ion association tendencies, classical gel electrophoresis and high-performance capillary electrophoresis in terms of separation efficiency, resolution, and speed, gas-sensing membrane materials and properties, properties and applications of different electrode types. **Analyze and Predict**: Mean ionic activity by comparing ionic strength and solubility using the MEKC method if elution time is given, separation of low molecular weight nitro compounds using the MEKC method and discuss elution order. **Evaluate and Interpret**: Effectiveness of biocatalytic membrane electrodes for determining BUN, value of the transfer coefficient in given data, nature of voltammogram, direction of scan, reversibility, and charge transfer mechanism. **Analyze and Evaluate**: Factors influencing overvoltage, current density, pH, and temperature, different theories of overvoltage and

		their applicability to electrochemical systems, slow processes in electrode reactions such as bubble formation, ion discharge, and proton transfer, effect of complex formation and dissolved oxygen on electrochemical reduction processes. **Interpret and Analyze**: Polarograms to determine diffusion currents and half-wave potentials, cyclic voltammograms to determine reversible, irreversible, and quasi-reversible charge transfer processes, diagnostic criteria for identifying different charge transfer mechanisms in cyclic voltammetry, voltammograms, peak current, electrode size, scan rate, and capacitance current.
LO5	Create	**Synthesize and Understand**: Interfacial electrochemistry comprehensively by integrating information from various models and theories. **Develop and Improve**: Strategies to minimize overvoltage and enhance the efficiency of electrochemical processes using theoretical principles and experimental data. **Design and Propose**: Experimental setups for specific electrophoretic separations based on principles of different electrophoretic modes, innovative modifications, or improvements to electrophoretic techniques by using data from different sources. **Optimize and Experiment**: Protocols for optimizing electrophoretic conditions including buffer composition, voltage gradients, and temperature control to achieve desired separation outcomes, experimental procedures for conducting polarographic experiments. **Explore**: Potential applications of potentiometry in new areas or applications through experimental design, and strategies to minimize or eliminate sources of polarization in electrochemical cells.
LO6	Evaluate	**Evaluate**: Strengths and limitations of the Debye-Hückel theory in explaining electrolyte behavior, the significance of ion association phenomena in understanding and predicting solution properties, strengths and limitations of Helmholtz-Perrin, Gouy-Chapman, and Stern models in describing the electrical double layer. **Critically Assess**: The factors influencing overvoltage and their impact on the efficiency of electrochemical processes, the advantages and disadvantages of capillary electrochromatography and micellar electrokinetic capillary electrophoresis compared to

		other modes of electrophoresis, the role of each component in electrophoretic setup for achieving optimal separation performance the potential applications and limitations of various electrophoretic techniques in different fields. **Evaluate and Critique**: The advantages and limitations of each type of electrode in voltammetry, reliability and accuracy of potentiometric measurements using different electrode types, experimental procedures involving potentiometric techniques. **Assess and Conclude**: Given data to justify the reversibility of a reaction and adherence to the correct electrochemical procedure, suitability of different types of mercury electrodes for specific electrochemical applications, accuracy and precision of concentration determination using polarography, significance of polarographic parameters in electrochemical analysis, reliability of experimental results obtained from polarographic experiments, appropriate voltammetric technique for specific analytical tasks based on advantages and limitations. **Critically Evaluate**: Effectiveness of electrochemical analysis at a DME and other solid electrodes.

Semester	III
Paper code	CH9425
Paper title	SOLID STATE CHEMISTRY
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text underlined, bold and in italics correspond to self-study.

2. Text within parentheses and italics correspond to recall/review.

1. GENERAL METHODS OF SYNTHESIS OF SOLIDS (5 + 1) hours

High temperature solid state synthesis; precursor methods; flux synthesis; combustion synthesis; chemiedouce (soft chemistry) methods; topotactic reactions; ***precipitation (including co-precipitation, and homogeneous precipitation),*** hydrothermal synthesis; sol-gel synthesis, advantages and disadvantages of solid state synthesis methods, application of product/s obtained using the above synthesis methods.

2. GEOMETRIC CRYSTALLOGRAPHY (12 + 2) hours

Crystalline and amorphous states of matter (recall). Periodicity in crystals. ***Seven crystal systems with unit cell parameters and essential symmetry elements-axis of symmetry, plane of symmetry, centre of symmetry.*** Symmetry elements and symmetry operations. Pure rotation axis, roto-inversion, roto-reflection axes, screw axes, glide planes. Derivation of non-occurrence of five-fold rotation axis. Combination of symmetry operations – Euler's construction (inter-axial angles) and its application to the general formula of the type A.B = C. Plane lattices, space lattices, point groups and space groups. Number of point groups in each crystal system, crystal classes. Stereographic projections of the following point groups: 222, 32, 422, 622, 23, 432 (Supporting the interfacial angles Euler's construction); space group representation – Hermann-Maugin symbols of some selected space groups.

3. CRYSTAL STRUCTURES OF SOME REPRESENTATIVE SYSTEMS: 3 hours

Olivines; corundum, ilmenite and $LiNbO_3$; garnets; K_2NiF_4 and Ruddlesden-Popper phases.

4. X-RAY DIFFRACTION **(11 + 2) hours**

Generation of X-rays, ***Bragg's equation and Bragg's method, Miller indices, unit cell parameters.*** X-ray structural analysis of solid substances: powder diffraction pattern of primitive, face-centered and body centered cubic lattices, indexing of reflections – graphical method and trial and error method, identification of space groups from systematic absences (space group extinctions). The concept of reciprocal lattice and construction of Ewald's sphere, derivation of Bragg's law from reciprocal lattice, structure factor and its relation to intensity, intensities from atomic positions for BCC and FCC lattices. Phase problem - heavy atom (Patterson's) method, introduction to the principles of direct methods of phase determination. Electron density function and electron density maps.

5. ELECTRON AND NEUTRON DIFFRACTION **2 hours**

Principles of electron and neutron diffraction; comparison with X-ray diffraction and applications.

6. DEFECTS IN SOLIDS **(3 + 1) hours**

Point defects – Schotky and Frenkel defects, ***colour centers and non-stoichiometric defects***. Line defects – edge dislocation and screw dislocation. Plane defects – grain boundary and stacking faults. Diffusion in solids, Fick's law.

7. PHASE TRANSITIONS IN SOLID **2 hours**

Definition and classification; first and second order phase transitions with examples.

8. ELECTRICAL AND MAGNETIC PROPERTIES OF SOLIDS **(14 + 2) hours**

Band theory: electron in periodic potential; Bloch theorem; Kronig–Penny model (derivation excluded); band structure – extended, reduced and repeat zone representation; Brillouin zones; DOS plots; metals, semiconductors and insulators. Properties of metals – ***metal-metal junction, thermoelectricity.*** Semiconductors – intrinsic and extrinsic semiconductors, Fermi levels of intrinsic, n-type and p-type semiconductors, electrons and holes, ***metal-semiconductor junction, p-n junction.*** Insulators – dielectric properties, piezoelectric effect, ferroelectricity, ferroelectric transitions in $BaTiO_3$, ionic conduction, electric breakdown. Magnetic properties of solids – paramagnetism, diamagnetism, ferromagnetism and anti-ferro magnetism – M vs H and χ vs T curves.

REFERENCES:

1. Introduction to solids, L.V. Azaroff, Indian Edn., Tata-McGraw Hill Publishing Company, New Delhi, 2001.
2. Fundamentals of Crystallography, C. Giacovazzo, International Union of Crystallography, 3rd Edn., Oxford University Press, 2011.
3. Elements of X-Ray Diffraction, B. D. Cullity, S.R. stock, 3rd Edn., Pearson Education India, (2014).

4. The Basics of Crystallography and Diffraction, C. Hammond, International Union of Crystallography, Oxford University Press, Oxford, 2015.
5. Solid State Chemistry and its Applications, A.R. West, Student Edition, John Wiley and Sons, 2014.
6. A Basic Course in Crystallography - J. Tareen and TRN Kutty, Universities Press, 2001.
7. Principles of the Solid State - H.V. Keer, 3rd Edn., Wiley Eastern Ltd., 2017.
8. Solid State Chemistry, D.K. Chakraborty, 2nd Edn., New Age International Publishers, 2010.
9. An Introduction to X-Ray Crystallography, M.M. Wolfson, 2nd Edn., Cambridge University Press, 2010.
10. Crystal Structure Analysis for Chemists and Biologists, J.P. Glusker, M. Levis and M. Ross, Wiley-VCH, 1996.
11. X-Ray Structure Determination – G.H. Stout and L.H. Jensen, 2nd Edn., Wiley-Interscience, 1989.
12. Solid State Physics- S. L. Gupta and V. Kumar, K. Nath and Co, Meerut, 2018.

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

LO1	Remember	Recall differences between amorphous and crystalline materials, concepts, laws, theorems, relationships, basic principles of X-ray diffraction Define the symmetry elements of a crystal, stereographic projection, plane lattices, space lattices, point groups and space groups, phase problem in X-ray diffraction, first order phase transition and second order phase transition with examples. Describe high temperature solid-state reactions, hydrothermal reactions, solvothermal synthesis, precursor methods; flux synthesis; combustion synthesis; chemiedouce (soft chemistry) methods; topotactic reactions
LO2	Understand	Explain periodicity in crystals, generation of X-rays, concept of reciprocal lattice, principles of electron and neutron diffraction, various methods to overcome the phase problem in XRD, electron density function and electron density maps, Bloch theorem; Kronig–Penny model, electronic structure theories and band theory, extended, reduced and repeat zone representation band structures, electronic structure theories and band theory Distinguish/differentiate between any two types of solid-state synthesis, the types and effects of defects in crystalline solids, including point defects, line defects, and plane defects, between ferroelectric and piezoelectric materials, between edge dislocation

		and screw dislocation Identify the similarities between K_2NiF_4 and Ruddlesden-Popper phases Describe the electronic properties of solids such as metals, insulators, and semiconductors, magnetic and electrical properties of solids, including diamagnetism, paramagnetism, ferromagnetism, and superconductivity, stereographic projections of selected point groups Illustrate structures of olivines; corundum, ilmenite and $LiNbO_3$ Derive non-occurrence of five-fold rotation axis in crystals, Braggs' law using concept of reciprocal lattice, Identify crystals with its symmetry using Hermann-Maugin symbols
LO3	Apply	Calculate inter-axial angles between the symmetry elements using Euler's construction Apply X-ray diffraction data to identify unknown crystalline substances, Brillouin zones to understand conductors and insulators
LO4	Analyze	Relate the symmetry elements with the periodicity of crystal, crystal structure and X-ray diffraction, structure factor and its relation to intensity in X-ray diffraction Compare and contrast electron, neutron and X-ray diffraction Analyze diffraction patterns to extract possible information about the crystal structure, the research gaps in different types of solid state synthesis
LO5	Create	Formulate structure factor and justify the intensity for the diffraction pattern from given atomic positions of a crystal
LO6	Evaluate	Justify the number of point groups in each crystal system, crystal class, the absences of certain intensities in relation to the lattice type Assess the possible combination of symmetry operations, the X-ray diffraction and assign the (h k l) values

Semester	III
Paper Code	CH9P1
Paper Title	APPLIED ANALYSIS – I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Inorganic Chemistry **11 sessions**

1. Non-aqueous titration
2. Analysis of alloy (Steel - Cr, Fe or other alloys) (2 sessions)
3. Analysis of soil (Cation exchange capacity and organic matter) (2 sessions)
4. Ion exchange Chromatography (Zn & Cd) (2 sessions)
5. Solvent extraction (Estimation of Fe III)
6. Determination of metal to ligand ratio by Job's method
7. Preparation of Ionic liquids
8. Preparation of graphite- intercalated compounds (RBPT)

REFERENCES:

1. Text book of Quantitative Inorganic Analysis, A.I. Vogel, 5th Edn., ELBS,1989.
2.Advanced Physicochemical Experiments, Rose and Isaac Pitman, 1st Edn., Pitman publishers, 1964.
3. A handbook of Soil Analysis, Tarafdar J.C, and B.K.Yadav, Agrobios publication, 2016.
4. Analytical Chemistry-An introduction; Skoog, West, Holler and Crouch, 10th Edn., Cengage learning India Pvt Publishing, 2022.
5. Experiments in Environmental chemistry, P.D. Vowels and D.W. Connel, Pergamon, 2013.

Learning outcomes: At the end of the practical, students will be able to:

LO1	Knowledge	Define nonaqueous titration Identify nonaqueous solvents used in titration Outline methodology for nonaqueous titrations Recall the principle of non-aqueous titration

		Give the chemical reactions involved in various titrations
LO2	Understand	Extrapolate redox titration to estimate iron and chromium in steel Explain the importance of calibration and standardization procedures in titrations, the theoretical principle of Job's method Describe the role of each reagent in the various volumetric estimations
LO3	Apply	Employ experimental techniques specific to ion exchange chromatography, including column packing, sample loading, elution optimization, and detection methods Choose synthetic techniques specific to the preparation of ionic liquids, including the selection of appropriate cations and anions, reaction conditions, and purification methods Demonstrate skills in sample preparation techniques tailored to solvent extraction Apply Job's method to determine the stoichiometry of metal-ligand complexes
LO4	Analyze	Analyze experimental data obtained from volumetric estimations and use it to determine the concentration of unknowns in a sample
LO5	Evaluate	Evaluate various techniques for determining the cation exchange capacity of soil samples Recommend suitable techniques for the characterization of synthesized compounds
LO6	Create	Design suitable techniques for the preparation of graphite-intercalated compounds by RBPT

Semester	III
Paper Code	CH 9P2
Paper Title	APPLIED ANALYSIS – II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Experiments in Biochemistry **11 sessions**

1. Estimation of rancidity in a sample of butter.
2. Estimation of BOD and COD of a sample.
3. Extraction of caffeine from tea leaves and characterization using IR, UV, and NMR spectrometer.
4. Estimation of glucose in serum.
5. Estimation of sulpha drug using spectrophotometer.
6. Estimation of RNA using spectrophotometer.
7. Estimation of cholesterol in serum.
8. Gel electrophoresis - separation of proteins.
9. Agarose gel electrophoresis - separation of RNA/DNA
10. Separation, purification and characterization of protein from plant sample.
11. Any other suitable experiments / RBPT.

REFERENCES

1. Vogel's Textbook of Practical Organic Chemistry, Furniss, 5th Edn., Pearson India, 2003.
2. Practical Clinical Biochemistry, H. Varley, 4th edition, CBS Indian edition, 2005.
3. An Introduction to Practical Biochemistry, David Plummer, 5th Edn., McGraw Hill Education, 2017.
4. Laboratory Manual in Biochemistry, J. Jayaraman, 2nd Edn., New Age International Private Limited, 2011.

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

LO1	Knowledge	**Define**: Rancidity, BOD, COD **Mention**: The key steps involved in preparing a tea leaf extract for caffeine analysis, the equipment and reagents required for glucose estimation, the names and functions of commonly used reagents and equipment in protein purification **Draw**: The structure and identify the characteristic functional groups present in caffeine, structure of the sulfa drug being analyzed **Recall**: The basic principles of glucose estimation in serum **List**: The components of a typical gel electrophoresis setup, including the gel matrix, buffer system, and electrodes, the factors that influence the migration of proteins in an electric field
LO2	Understand	**Explain**: The basic principles of spectrophotometry and colorimetric techniques and its application in nucleic acid quantification, glucose estimation; principle involved in the solvent extraction method used in the isolation of caffeine from tea leaves; principles of gel electrophoresis and its application in separating biomolecules such as proteins, the chemical processes involved in the development of rancidity in butter, the clinical significance of serum cholesterol, the significance of rancidity, BOD, COD, the basic principles of caffeine extraction from tea leaves using a solvent extraction method, the biochemical basis of glucose estimation, including enzymatic and chemical methods, the biochemical basis of glucose estimation, including enzymatic and chemical methods, the significance of measuring glucose levels in serum for assessing metabolic health **Identify**: Functional groups in organic molecules based on IR spectra **Describe:** The principles behind spectrophotometric and colorimetric techniques used in glucose estimation; the principles of different methods for cholesterol estimation in serum, such as enzymatic assays or colorimetric reactions; basic principles of protein separation, purification, and characterization techniques, the principles underlying various protein separation techniques, such as chromatography,

		electrophoresis, and precipitation, the biochemical and chemical processes involved in BOD and COD determination **Differentiate**: Between BOD and COD, between native polyacrylamide gel electrophoresis (PAGE) and denaturing PAGE in terms of protein structure and separation conditions **Discuss**: The factors that may influence the accuracy and reliability of RNA quantification using spectrophotometry Explain various protein extraction methods from plant tissues, the mechanism by which proteins migrate through a gel matrix under the influence of an electric field, the absorbance spectrum of the sulfa drug to determine the optimal wavelength for measurement
LO3	Apply	**Identify and apply**: Appropriate methods for detecting rancidity in butter samples **Extract:** Caffeine from tea leaves **Draw and interpret**: Calibration curves and standard solutions to accurately quantify glucose concentrations in serum **Demonstrate:** The use of appropriate instruments and equipment for glucose estimation assays **Prepare:** Solutions of the sulfa drug for analysis, RNA samples for spectrophotometric analysis, serum samples for cholesterol estimation, prepare protein samples for gel electrophoresis, including sample loading and buffer preparation, plant samples for protein extraction, including sample homogenization and preparation of extraction buffers **Choose**: Appropriate gel concentrations for gel electrophoresis and running conditions for separating proteins of interest **Demonstrate:** Proficiency in running gel electrophoresis experiments and handling protein samples safely **Use:** Chromatography columns, electrophoresis gels, and other equipments for protein purification
LO4	Analyze	**Predict**: Susceptibility to rancidity based on the chemical composition of butter **Explain:** Choice of solvent, extraction time and temperature for efficient caffeine extraction **Optimize:** Glucose estimation, cholesterol estimation assays such as sample preparation, reagent quality and instrument calibration

		Compare: The roles of BOD and COD in indicating organic pollution in water bodies **Analyze**: The results of gel electrophoresis experiments to interpret the migration patterns of proteins in the gel **Compare and contrast**: The separation efficiencies of different gel types and electrophoresis conditions for separating proteins, different protein purification methods for isolating target proteins from plant samples **Interpret**: The results of protein separation experiments to assess the purity and yield of purified protein fractions, chromatograms, electrophoresis gels and other separation profiles to identify target proteins and contaminants
LO5	Evaluate	**Compare**: The various estimation methods of butter samples based on the type and extent of rancidity, the IR spectra of caffeine with spectra of other compounds to distinguish caffeine from similar molecules, different methods of glucose estimation and evaluate their advantages and limitations **Interpret**: The relationship between BOD and COD with the amount of organic matter present in water **Assess:** The suitability of spectrophotometric analysis for quantifying RNA in various experimental contexts such as gene expression studies or RNA isolation protocols, potential sources of error in cholesterol estimation assays and propose strategies to minimize them **Critique**: The reliability and accuracy of various cholesterol estimation methods in clinical practice, potential sources of error in gel electrophoresis experiments such as improper gel preparation or incomplete denaturation of proteins, and propose strategies to minimize them, potential sources of error in protein purification experiments such as incomplete extraction or nonspecific binding, and propose strategies to minimize them **Evaluate**: The reliability and reproducibility of gel electrophoresis as a method for protein separation and analysis, the effectiveness of protein extraction and purification protocols in achieving the desired level of protein purity and yield. **Interpret**: Chromatograms, electrophoresis gels and other

		separation profiles to identify target proteins and contaminants Compare and contrast the efficiency and specificity of different protein purification methods for isolating target proteins from plant samples
LO6	Create	**Design:** An experiment to investigate the effectiveness of various antioxidants in preventing rancidity in butter, an experiment to investigate the impact of different pollutants on BOD and COD levels in water in terms of concentration and exposure time, an experimental protocol to optimize the extraction conditions for caffeine from various sources in terms of solvent choice and extraction parameters, an experimental protocol to optimize the conditions for cholesterol estimation in serum samples in terms of sensitivity, specificity and reproducibility, an experimental protocol to optimize the conditions for separating proteins of interest using gel electrophoresis including gel composition, running parameters and staining methods, an experimental protocol to optimize the conditions for protein extraction and purification from a specific plant sample. **Develop**: A monitoring plan for assessing BOD and COD levels in a local water body, a standardized procedure for quality control and quality assurance in glucose estimation including validation of results and proficiency testing, a standard operating procedure (SOP) for quality control and validation of spectrophotometric methods used in sulfa drug analysis and RNA quantification, a standardized procedure for quality control and quality assurance in cholesterol estimation, a standard operating procedure (SOP) for quality control and validation of gel electrophoresis experiments and protein purification

Semester	III
Paper Code	CH 9P3
Paper Title	ADVANCED METHODS OF ANALYSIS-I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

List of Experiments **11 sessions**

1. Estimation of Cd/Zn/Mg in a given sample using AAS
2. Separation and identification of organic compounds using GC
3. Analysis of components of essential oils using GC
4. Estimation of caffeine using HPLC
5. Estimation of citric acid in fruit juice using HPLC
6. Thermal analysis (TGA/DTA) of a given sample
7. Estimation of a dye by fluorimetry
8. Analysis of emission spectrum of tris(8-hydroxyquinolinato) aluminium(III) (AlQ3)
9. Estimation of bandgap of a semiconductor from diffuse reflectance spectrum
10. Determination of water content of a sample by Karl-Fischer titration
11. Any other experiment/Viva

REFERENCES:

1. Principles of Instrumental Methods of Analysis, 7th Edn., D. A. Skoog, F. J. Holler, S. R. Crouch, Cengage India Pvt. Ltd., 2020.
2. Practical Instrumental Analysis, S. Petrozzi, Wiley-VCH Verlag & Co., 2013.
3. Instrumental Methods of Chemical Analysis, V.K. Ahluwalia, Springer, 2023.
4. Chemical Analysis, 2nd Edn., F. Rouessac, A. Rouessac, John Wiley & Sons Ltd, 2007.
5. Instrumental Methods of Analysis, 7th Edn., H. H. Willard, L. L. Merritt Jr, J. A. Dean, Wardsworth Publishing Company, 2001.

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

LO1	Knowledge	Recall the principles of AAS, HPLC, GC, Fluorescence spectroscopy
LO2	Understand	Explain principles of AAS, HPLC, GC, Fluorescence spectroscopy
LO3	Apply	Apply the principles of AAS, HPLC, GC, Fluorimetry and Karl-Fischer titrations for the respective estimations/analysis
LO4	Analyze	Compare and contrast the GC and HPLC analysis for a given compound
LO5	Evaluate	Assess various methods of estimation of the citric acid content in a given fruit juice sample
LO6	Create	Test new methods/protocols for the estimation of given sample using AAS, HPLC, GC, Fluorimetry and Karl-Fischer titrations

Semester	III
Paper Code	CH9P4
Paper Title	ADVANCED METHODS OF ANALYSIS-II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Flame Photometer experiments

1. Estimation of sodium/potassium/lithium by flame photometer. (1 session)
2. Estimation of alkali metals in a given mixture by flame photometer. (1 session)

Spectrophotometer experiments

3. Estimation of caffeine using UV spectrophotometer. (1 session)
4. Estimation of Ni in tea powder. (1 session)
5. Estimation of chloride in pharmaceutical products. (1 session)
6. Estimation of mixture of Mn and Cr. (1 session)

Polarimeter experiments

7. Determination of unknown amount of sucrose in a given solution by polarimeter. (1 session)

Electroanalytical experiments

8. Estimation of copper by potentiometry. (1 session)
9. Estimation of sulphides in water sample by potentiometry. (1 session)
10. Estimation of a mixture of chloride and iodide by potentiometry. (1 session)
11. Studying electrochemically reversible ferrocyanide-ferricyanide system using cyclic voltammetry. (1 session)
12. Determination of strength of acid/base using auto-titrator in aqueous or non-aqueous media. (1 session)

Turbidimeter experiment

13. Estimation of sulphate in water sample using turbidimeter. (1 session)

Residue of ignition experiment

14. Estimation of metal using residue of ignition method. (1 session)

REFERENCES:

1. Vogel, A. I. A text book of Quantitative Analysis, ELBS 1986.

2. Khosla, B. D.,Garg, V. C. and Gulati, A. Senior Practical Physical Chemistry, R. Chand and Co. (2011).

3. Garland, C. W., Nibler, J. W. and Shoemaker, D. P. Experiments in Physical Chemistry, 8th Ed, McGraw-Hill: New York (2003).

4. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman and Co., (2003).

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

LO1	Knowledge	**Recall**: i) the principle of flame photometry and its application in detecting alkali metals ii) the principles of electrochemistry and the definitions of terms such as oxidation, reduction, cyclic voltammetry, ferrocyanide, and ferricyanide iii) the principles of UV spectrophotometry iv) the fundamental principles of potentiometry and its application in chemical analysis v) principles of auto-titrator **Remember**: i) the specific emission wavelengths for sodium, potassium, and lithium ii) the steps involved in the estimation of copper using potentiometry iii) the experimental procedure and safety protocols involved in conducting cyclic voltammetry experiments iv) the operating procedures for flame photometer v) the operating procedure for spectrophotometer vi) the operating procedure for polarimeter vii) the operating procedure for UV-Vis instrument viii) the operating procedure for electroanalytical techniques ix) the operating procedure for auto-titrator. **Identify**: i) the characteristics of caffeine absorption in UV spectra ii) the significance of nickel analysis in food products, particularly in tea powder iii) the principles and methods used to estimate chloride in pharmaceutical products iv) the appropriate chemical reagents and techniques used in the estimation of Mn and Cr v) the necessary equipment and reagents for the experiment vi) principles and methods required for auto-titrator. Outline the standardization procedures for the reagents and equipment used. **List** the characteristic wavelengths by atoms and ions in a flame photometer.
LO2	Understand	**Explain**: i) the principle behind flame photometry and the emission spectra of alkali metals ii) the concept of UV absorption and how it

		relates to caffeine concentration iii) the principles behind the analytical methods used to estimate nickel in tea powder iv) the chemical reactions involved in the determination of chloride ions in pharmaceutical samples v) the underlying theory of potentiometry and how it applies to estimating copper ions vi) the principles of calibration and standardization in potentiometric analysis vii) the importance of calibration curves and standard solutions in potentiometric analysis viii) the chemical reactions involved in detecting and quantifying sulfides in water samples ix) the concept of reversible redox reactions and how they are observed in the ferrocyanide-ferricyanide system x) the concept of auto-titrator and how to develop a method for aqueous and non-aqueous titration. **Describe**: i) the factors influencing the sensitivity and selectivity of flame photometry ii) the process of preparing samples for UV analysis and the importance of calibration iii) the process of preparing samples for polarimeter experiment iv) the process of preparing samples for auto-titrator **Interpret**: i) UV spectra to identify caffeine peaks ii) the chemical reactions and instrumental techniques involved in nickel determination iii) the significance of specific reagents and techniques employed in the determination of chloride ions iv) the principles behind the analytical methods employed in estimating the mixture of Mn and Cr v) the cyclic voltammogram obtained from the experiment, including the shapes of the curves and the significance of peak potentials vi) the results in terms of sulfide concentration in the water sample vii) results and data in auto-titrator. **Comprehend**: i) the significance of electrode potential in determining copper concentration ii) how the potentiometric method measures the concentration of sulfide ions iii) the theory behind the determination of concentrations from potentiometric data. **Summarize** the procedures involved in the experiment, including the preparation of samples and standards in estimating the mixture of Mn and Cr. **Discuss** the underlying theory of potentiometry and how it applies to estimating copper ions. **Outline** the difference in behavior between chloride and iodide ions in potentiometric titrations. **Understand**: i) the fundamental principles of polarimetry, including the

		interaction of polarized light with optically active substances and the measurement of optical rotation ii) operating a polarimeter, including instrument setup, calibration, and alignment of optical components for accurate measurements iii) the kinetics of electrode reactions, including mechanisms of electron transfer, rate constants, and factors affecting reaction rates, and apply kinetic principles to interpret electroanalytical data iv) the basic principles of spectrophotometry, including Beer-Lambert Law, absorption spectra, and the relationship between absorbance, transmittance, and concentration v) to operate a spectrophotometer, including knowledge of instrument components, setup procedures, and basic troubleshooting techniques vi) the process of calibration and standardization in spectrophotometry, including preparing calibration curves, determining the linear range, and establishing the detection limits for analytes of interest
LO3	Apply	**Utilize:** i) the flame photometer to measure the emission intensity of alkali metals accurately ii) the UV spectrophotometer to measure the absorbance of caffeine solutions accurately iii) appropriate calibration curves and standard solutions to calculate the concentrations of Mn and Cr in the unknown sample iv) knowledge of stoichiometry and titration techniques to calculate the concentrations of chloride and iodide ions in the mixture **Apply**: i) calibration methods to determine the concentration of alkali metals in a given mixture ii) appropriate sample preparation techniques to extract nickel from tea powder effectively iii) appropriate sample preparation techniques to ensure accurate estimation of chloride concentration in pharmaceutical products iv) the techniques learned to perform the estimation of copper accurately v) mathematical calculations to determine the concentration of copper in the sample vi) knowledge of electrochemistry to predict the behavior of the ferrocyanide-ferricyanide system under different experimental conditions vii) principles of data analysis to extract relevant information from the cyclic voltammogram, such as peak potentials and peak currents viii) the knowledge in the instrument setup, calibration, and optimization of parameters such as flame temperature and fuel-to-oxidant ratio in case of a flame photometer. **Demonstrate** proficiency in handling potentiometric equipment and reagents.
LO4	Analyze	**Analyze**: i) the correlation between emission intensity and alkali metal

		concentration using calibration curves ii) the experimental data obtained during the estimation of sulfides iii) the relationship between absorbance and caffeine concentration using calibration curves iv) experimental data obtained from the nickel estimation to calculate the concentration of nickel in the tea powder v) the experimental data obtained during the estimation process vi) the data to determine the equivalence point vii) experimental data to determine kinetic parameters such as peak potential separations and peak currents viii) the concentration of targeted elements quantitative analysis of optically active substances using polarimetry, including calibration curve construction, sample measurement, and data analysis to determine concentration or specific rotation ix) the strength of unknown acid/base in aqueous or non-aqueous solution **Interpret** experimental data to calculate the chloride concentration in the pharmaceutical samples. **Compare and contrast** the behavior of the ferrocyanide-ferricyanide system with other electrochemically reversible redox couples.
LO5	Create	**Create**: i) educational materials or presentations to explain the principles and applications of flame photometry in alkali metal analysis in various samples ii) educational materials or presentations to explain the principles and applications of UV spectroscopy in various samples iii) comprehensive reports or presentations summarizing the experimental procedure, results, and conclusions. **Design and execute** flame photometry experiments to address specific research questions or objectives, considering factors such as sample matrix complexity and analyte concentration range.
LO6	Evaluate	**Assess**: i) the reliability of flame photometry as a method for estimating alkali metals compared to alternative techniques ii) the reliability of the UV spectrophotometer method for caffeine estimation compared to other methods iii) the potential health risks associated with the observed nickel levels in tea powder, considering consumption patterns and regulatory standards iv) the compliance of the chloride concentration in pharmaceutical products with regulatory standards and specifications, considering the impact on product quality and safety. **Compare and contrast** the advantages and limitations of different analytical methods for estimating the concentrations of Mn and Cr in mixtures. **Evaluate**: i) the reliability and accuracy of the estimation method used ii) the reliability of the potentiometric method for the determination of

		chloride and iodide ions. **Critically assess**: i) the limitations of potentiometry in determining copper concentration ii) the limitations and advantages of potentiometry in detecting sulfides in water samples **Compare** the advantages and limitations of potentiometric analysis with other analytical techniques.

FOURTH SEMESTER

THEORY PAPERS

Semester	IV
Paper Code	CH 0125
Paper Title	APPLIED ANALYSIS
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. BIOPOLYMERS **3 hours**

Determination of size, shape and molecular weight by sedimentation, diffusion and viscosity methods.

2. PROTEIN ANALYSIS **(12 + 2) hours**

Protein purification: protein isolation, solubility of proteins, ***chromatographic separations***, ***electrophoresis and centrifugation***. ***Analysis and determination of protein structure: primary structure,*** protein modification, secondary structure, globular and fibrous proteins, tertiary structure, quaternary structure. Techniques for study of biomolecules (principle and interpretation of data to characterize the biomolecule) – mass spectrometry (MALDI/ SELDI), confocal microscopy, microarrays, flow cytometry, microcalorimetry, differential scanning calorimetry, ELISA, RIA, FACS, Northern, Southern, Western blots, NMR, electrophoresis, CD, ORD, X-Ray crystallography.

3. NUCLEIC ACID ANALYSIS **(3 + 2) hours**

Analysis and determination of structure of nucleic acids: ***primary structure, secondary structures, denaturation, renaturation, tertiary structure***. Chemical synthesis of polynucleotides. Recombinant DNA: cloning, DNA libraries, PCR and recombinant DNA technology. A brief account of the application of recombinant technology in different disciplines - industry, medicine and forensics.

4. FOOD ANALYSIS **(4 + 2) hours**

Analysis of common adulterants in foods. Food additives: monosodium glutamate. Food preservatives: sodium benzoate, sodium sulphite. Milk and milk products-alcohol test, fermentation test, dye reduction tests (methylene blue and resazurin), phosphatase test for pasteurisation, ***estimation of added water in milk***. Beverages- caffeine and chicory in coffee, methanol in alcoholic drinks. Estimation of saccharin, coal tar dyes and aflatoxins in foods. Pesticide analysis in food products: phospho- and chloro- pesticides.

5. ANALYSIS OF DRUGS AND POISONS (4 + 2) hours

***Classification of drugs, characterisation of common drugs: analgesics - aspirin; expectorants – benadryl; vitamins - vitamin C; sedatives - diazepam; antibiotics - penicillin, chloramphenicol; cardiovascular – sorbitrate*.** Determination of barbiturate drugs (phenobarbital) in drug samples, and its clinical significance. Analysis of snake venom poison: phospholipases, hyaluronidase, toxic peptides.

6. CLINICAL CHEMISTRY 3 hours

Blood analysis: serum electrolytes, serum proteins, blood glucose, blood urea nitrogen, uric acid, and blood gas analysis. Enzyme analysis: assay of alkaline phosphatase, assay of Serum glutamic oxaloacetic transaminase and Serum glutamic pyruvic transaminase and their clinical significance, isoenzymes of lactate dehydrogenase, aldolase. Metal deficiency and disease: estimation of calcium, iron, and copper.

7. LIPID ANALYSIS 3 hours

Edible oils - qualitative tests for purity, estimation of rancidity, tests for common adulterants in edible oils.

8. POLLUTION ANALYSIS 8 hours

Air pollution: principles and methods of sampling; a survey of reactions and methods involved in the determination of carbon monoxide, sulphur oxides, nitrogen oxides, hydrocarbons and particulates. Tolerance limits. Fuel Analysis and emissions: ultimate and proximate analysis of coal, quality of liquid fuels - octane number, cetane number and carbon residue.

Water pollution: objectives of analysis; parameters of analysis: colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen; heavy metal pollution: public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental techniques for the analysis of heavy metals in aqueous systems.

9. SOIL ANALYSIS 4 hours

Chemical properties of soil - types of soil colloids, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination. Acid soils - types of soil acidity, liming, measurement of pH and conductivity of soil. Saline and alkaline soils. Analysis of major constituents of soil - organic matter, nitrogen, sulphur, sodium, potassium and calcium.

10. RADIOACTIVE POLLUTION **4 hours**

Detection and monitoring of radioactive pollutants; methods for the safe disposal of radioactive waste. Dosimetry. Advantages and restrictions of radiotracer experiments, safety aspects.

11.DRUG DISCOVERY REGULATIONS **4 hours**

Preclinical toxicology testing and IND application: regulatory acts and regulatory bodies, main stages of preclinical toxicology testing-acute toxicity studies, repeated dose studies, genetic toxicity studies, reproductive toxicity studies, carcinogenicity studies and toxicokinetic studies.

REFERENCES:

1. Environmental pollution analysis, S.M. Khopkar, Wiley Eastern, 1993.
2. Principles of Biochemistry, David L Nelson and Michael M.Cox 8th Edn, Macmilan Learning, 2021.
3. Biochemistry, L. Stryer, 10th Edn., Macmillan Learning, 2023.
4. Biochemistry, Voet and Voet, 5th Edn., John Wiley, 2018.
5. Biophysical Chemistry Principles and Techniques, Upadhyay and Nath, Himalaya Publishing Company, 2016.
6. Experiments in environmental chemistry, P. D. Vowels and D. W. Connel, Pergamon, 1980.
7. Handbook on air pollution, Stern, APHA, 1980.
8. Principles of instrumental analysis, D. A. Skoog and West. Saunders College, 1980.
9. Food analysis, A. G. Woodman, McGraw Hill, 1971.
10. Milk and milk products, C. H. Eckles, W.B. Combs and H. Macy, Tata McGraw Hill, 1976.
11. Radioactivity introduction and history, Michael F L' Annunziata, Elsevier, 2007.
12. Air pollution control, a design approach, C. David Cooper, F. C. Alley, Waveland Press, 2011.
13. Practical clinical biochemistry, H. Varley, 4th edition [CBS] Indian edition, 1988.
14. Separation techniques in chemistry and biochemistry, Roy Keller, Marcel. Dekker, 1967.
15. Methods of soil analysis part I & II, C. A. Black et al (Edition), American Society of Agronomy, 1965.

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

LO1	Knowledge	Recall the sources, structures, metabolism and biological importance, deficiency of proteins nucleic acids and lipids Recognize various types of soil pollutants, their sources and pathways of contamination; food additives and preservatives; types and sources of radiation, potential health hazards of radioactive pollution
LO2	Understand	Explain the concept of selectivity and specificity in protein purification, different protein purification methods, concepts and applications related to recombinant DNA technology the principles and applications of various techniques for structural determination of proteins and nucleic acids, such as sequencing methods, Mass spectrometry, X-ray crystallography, NMR and confocal microscopy Compare fibrous and globular proteins, renaturation and denaturation, drugs and poisons, consequences of radioactive pollution - contamination of air, water, soil, and ecosystems, as well as bioaccumulation and biomagnification in food chains
LO3	Apply	Identify biomolecules based on the principles of various analytical methods such as SDS-PAGE, blotting techniques, microarrays, Flow cytometry, ELISA, RIA, DSC and microcalorimetry; natural and human-made sources of radioactive pollution, such as nuclear power plants, mining activities, medical facilities, and industrial processes Comprehend the potential health hazards associated with exposure to radioactive pollution
LO4	Analyse	Interpret experimental data obtained from various analytical techniques for biomolecules, food additives, drugs and poisons Assess adsorption, leaching, volatilization and degradations that influence the behavior and fate of pollutants in soil environments and assign for agricultural and construction purposes Correlate lipid intake, cholesterol levels, cardiovascular disease risk, obesity, diabetes and other metabolic disorders
LO5	Evaluate	Explore and assess the role of protein purification in the development of therapeutic proteins and diagnostic tools, national and international regulations and protocols governing the management and disposal of radioactive waste Develop methods for protein and nucleic acid structure

		determination, biopolymer characteristics, food adulteration detection kit, nutrition chart based on local food habits, pollution remediation strategies, soil quality improvement strategies, remediation techniques and technologies for radioactive contamination in different environment Prepare a manual to monitor environmental implications of food additives and preservatives, including their production, usage, and disposal, and explore strategies for minimizing their environmental footprint and promoting sustainable food systems. Propose methods for restoration of polluted soils
LO6	Create	Design dietary measures based on correlate local food habits to combat prevalent clinical deficiencies, nuclear reactors according to geographic locations Develop skills in assessing and managing risks associated with radioactive pollution, monitoring techniques, emergency response procedures, and strategies for minimizing exposure and contamination Integrate pest management, organic farming, soil conservation in rural and urban planning measures

Semester	IV
Paper code	CHDE 0225
Paper title	CHEMISTRY OF MATERIALS
Number of teachings hours per week	4
Total number of teachings hours per semester	60
Number of credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. INTRODUCTION **1 hour**

Importance of solids in technological applications, solids as materials.

2. MATERIALS CHARACTERISATION TECHNIQUES **14 + 1 hours**

Electron microscopy and related techniques: transmission electron microscopy, scanning electron microscopy, electron diffraction, electron energy loss spectroscopy, energy dispersive X-ray spectroscopy. Atomic force microscopy. Photoelectron spectroscopy and auger spectroscopy. Particle induced X-ray emission spectroscopy. Extended X-ray absorption fine structure. Porosity and surface area measurements by sorption- desorption – BET and BJH methods.

LAYERED SOLIDS AND POROUS MATERIALS **7+ 3 hours**

Layered solids***: <u>general structural features, classification, intercalation and deintercalation</u>***. Structure, composition, properties and applications of cationic clays, layered double hydroxides, layered chalcogenides and layered oxides. Polytypism in layered solids.

Microporous and mesoporous materials: structure, composition, synthesis, properties and applications of zeolites, zeotypes and ***<u>metal organic frameworks. Macroporous solids: Methods of preparation, properties and applications of opals and inverse opals</u>***.

3. SUPERCONDUCTORS **5 hours**

Definition, Meissner effect, type 1 and type 2 superconductors, features of superconductors, Frolich diagram, Cooper pairs, theory of low temperature superconductivity, high T_C superconductors.

3. SOME MATERIALS OF RECENT INTEREST **5 + 1 hours**

Multiferroics, giant and colossal magneto resistance (GMR, CMR) materials thermoelectric materials, topological materials, conducting polymers.

NANOMATERIALS **20 + 3 hours**

Nanoregime, properties at nanoregime- electronic structure of metals and semiconductors at nanoscale, quantum confinement, superparamagnetism of magnetic solids at nanoscale. Classification of nanomaterials.

Synthesis of nanocrystals: top-down vs bottom-up synthesis, dispersity, La Mer principle, capping agents, simple solution-based synthesis, inverse-micelle synthesis, ***spray pyrolysis, sol-gel, combustion,*** solvothermal and electrochemical synthesis.

Synthesis of thin films: physical vapour deposition – pulsed laser deposition and atomic layer deposition, chemical vapour deposition, electrodeposition.

Synthesis of 2D nanomaterials: mechanical, solvent-mediated, and chemical exfoliation. Use of PXRD, UV-visible and Raman spectroscopy in the characterization of nanomaterials. Nanocomposites: definition, different types, general methods of synthesis and applications. Carbon-based nanomaterials: structure, synthesis, properties and applications of fullerenes, carbon onions, carbon nanotubes and graphene.

Applications of nanomaterials: nanomaterials in energy conversion and storage; environmental amelioration applications; electronic and optoelectronic applications; theranostic and biological applications. ***Nanotoxicity***.

REFERENCES

1. Electronic absorption spectroscopy and related techniques by D. N. Sathynarayana, Universities Press (India) limited, 2001
2. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, 2nd Edn., Cambridge Univ. Press., 2010.
3. Molecular Sieves, Science and Technology Series, Karge, H. G. Ed Weitkamp, J. Ed Auroux, A Berlin Springer Verlag. Volume 6, 2008.
4. Nanoscale Materials in Chemistry, Kenneth J. Klabunde, John Wiley and Sons, 2000.
5. The Chemistry of Nanomaterials: Synthesis, Properties and Applications, C.N.R Rao, Dr. H. C Mult. Achim Muller, Prof. A. K. Cheetham, Wiley VCH 2004
6. Biomaterials Science, Buddy Ratner, Allan S Hoffmann, Jack E Lemons, Frederick JSchoen, B.D. Ratner, 2nd Edition, Academic Press, 2004.
7. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Guozhong Cao, Imperial College Press, 2004.
8. Hybrid Nanocomposites for Nanotechnology: Electronic, Optical, Magnetic and Biomedical Applications, Lhadi Merhari, Springer Publications, 2009.

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

LO1	Knowledge	Recall polytypism, cationic clays, layered double hydroxides, layered chalcogenides and layered oxides Define Meissner effect, ferroelectric, ferromagnetic, ferroelastic and multiferroic materials, CMR, GMR, thermoelectric materials, topological materials and conducting polymers, nanomaterials
LO2	Understand	Explain different microscopic techniques, the mechanism of electrical conductivity in conducting polymers Describe different spectroscopic characterization techniques for materials, features of superconductors, Cooper pairs, high Tc superconductors, properties of multiferroic, GMR and CMR, thermoelectric materials, topological insulators, the unique properties of nanomaterials compared to bulk materials, the different synthesis methods used to synthesize nanomaterials Compute porosity, pore volume Differentiate electron energy loss spectroscopy, energy dispersive X-ray spectroscopy, intercalation and deintercalation, macroporous, mesoporous and microporous materials, type 1 and type 2 superconductors Illustrate photoelectron process and auger electron emission, Frolich diagram Discuss theory of low temperature superconductivity
LO3	Apply	Calculate surface area of zeolites and mesoporous materials Draw primary, secondary and tertiary building units of zeolites Predict the observed ferromagnetic and ferroelectric phenomena based on multiferroic properties
LO4	Analyze	Classify Zeolites Compare and contrast SEM and TEM, cationic and anionic clays, opals and inverse opals, different types of multiferroic materials and their applications Examine experimental data from characterization techniques to draw conclusions about nanomaterial structure and properties Predict suitable materials for thermoelectric, topological, GMR effect based on their unique electronic and magnetic property Relate critical temperature, critical magnetic field, entropy and free energy of normal state and superconducting state.
LO5	Evaluate	Predict photoelectron and auger spectra of compounds. Interpret ESCA spectra of unknown compound.

		Differentiate different structures of doubly oxidized cystin. Assess the effectiveness of different synthesis techniques to produce nanomaterials with desired properties
LO6	Create	Synthesis of different zeotypes Develop novel approaches for improving the performance of multiferroic devices, innovative synthesis techniques for different class of nanomaterials

Semester	IV
Paper code	CHDE 0325
Paper title	GREEN CHEMISTRY AND DIVERSITY OF ITS APPLICATIONS
Number of teaching hours per week	4
Number of teaching hours per semester	60
Number of Credits	4

NOTE: 1. Text bold, italics and underline correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review.

1. SUSTAINABILITY AND PRINCIPLES OF GREEN CHEMISTRY 4 hours

Definition of sustainability, basic principles, models of sustainable development; three pillar model, sustainability issues, challenges to sustainability.

Green chemistry as one of the approaches to sustainability. 12 Principles of green chemistry: prevention of waste, less hazardous chemical synthesis, safer solvents and auxiliaries, use of renewable feed stock, catalysis, real time analysis for pollution prevention, atom efficiency, designing safer chemicals, design for energy efficiency, reduced derivatives, design for degradation, inherently safer chemistry for accident prevention.

2. USE OF ULTRASOUND AND MICROWAVE IN ORGANIC SYNTHESIS 3 hours

Use of ultrasound: instrumentation and the phenomenon of cavitation. Sonochemical esterification, oxidation and reduction. Use of microwave: introduction, reaction vessel and medium, specific effects, atom efficiency, advantages and limitations, N-alkylation and alkylation of active methylene compounds with aldehydes and amines.

<u>Diels-Alder reaction and oxidation of alcohols.</u>

3. MECHANOCHEMISTRY 5 hours

Definition of mechanochemistry. Mortar and pestle for organic synthesis. Ball milling as reactors for organic synthesis; factors which affect ball-milling reactions, advantages and disadvantages of ball-milling reactors.

Case study: **Solvent-free reactions of alkynes in ball mills:** Pd-catalysed Sonogashira cross coupling and Cu-catalyzed homo-coupling (Glaser reaction); Comparison of results to other solvent-free reaction published protocols, assessment of the reaction based on the variables, type of catalyst and base or reaction time. Evaluation of performance-based parameters (yield, selectivity, turnover number, TON, and turnover frequency, TOF), comparison with micro wave irradiation with respect to reaction time and TOF.

4. POLYMER SUPPORTED REAGENTS IN ORGANIC SYNTHESIS (4+1) hours

Introduction- structure of polymer supports, properties of polymer support, advantages of polymer supported reagents and choice of polymers.

Applications: substrate covalently bound to the support - synthesis of oligosaccharides, Dieckmann cyclisation. Use of Merrifield resin in peptide synthesis. Reagent linked to a polymeric material - synthesis of polymer bound per acid and its applications. ***Polymer supported catalytic reactions: preparation of polymer supported AlCl3, and application in acetal formation reaction***.

5. PHASE TRANSFER CATALYSIS (PTC) AND CROWN ETHERS (4+1) hours

Definition, mechanism of PTC, types of PTC reactions and advantages. Preparation of catalysts and their application in alkylation, oxidation and reduction reactions.

Crown ethers: general structure, nomenclature, features and nature of donor site. General synthesis of crown ethers. Synthetic applications: aromatic substitutions.

Generation of carbenes and alkylation

6. MULTICOMPONENT ONE-POT REACTIONS (4+1) hours

Meaning of one pot synthesis (mention of synonyms domino/cascade/ tandem reactions). Effective reactions for one-pot synthesis; reaction in which the intermediate compound is unstable, reaction in which the intermediate compound is hazardous, reactions in which there is equilibrium between intermediate compounds, reaction in which the starting compound is in equilibrium with the intermediate, ***reaction in which same reagents are employed in subsequent reactions; an example each.*** Restriction for one-pot reactions; reaction, solvent, amunt of reagent, e.g., Passerini, Ugi, Biginelli and Mannich reactions.

7. BIODEGRADABLE POLYMERS (2+1) hours

Definition, classification based on origin and method of production, examples. Biodegradable polymers derived from (i) petroleum sources (ii) renewable resources. Blends of biodegradable polymers. Drawbacks of natural fibers, surface modification-chemical and biological treatment. Application of biodegradable polymers.

End of life scenarios and degradation end products.

8. ORGANOCATALYSIS (12+1) hours

Introduction- types of organocatalyst, advantages, reusability.

Enamine catalysis: Aldol and Mannich type reactions, α-heteroatom functionalization, direct conjugate additions via enamine activation.

Iminium catalysis: cycloaddition reactions, 1,4-addition reactions, transfer hydrogen reactions, cascade reactions- total synthesis of natural products- tetrahydroquinoline alkaloids.
N-Heterocyclic Carbenes (NHC): Conjugate umpolung of α, β-unsaturated aldehydes for the synthesis of gamma-butyrolactone.
Hydrogen bonding networks - epoxidation of olefins and Baeyer–Villiger oxidation of ketones.
Supported organocatalyst and Ionic liquid organocatalyst.
Precursors and generation of NHC.

9. GREEN CHEMISTRY PRACTICES IN PHARMACEUTICAL INDUSTRY (10+1) hours

Solvent categories in pharmaceutical process development and greenness factor.
Supercritical fluids and applications.
Water as solvent: under pressure enabling reactions at high temperature, in ring closure reactions under PTC conditions, dehydrohalogenation under PTC conditions.
Solvent free reactions: e.g., Biginelli reaction.
Case studies: (i) Convergent synthesis of Sildenafil citrate (ii) Comparison of routes between the old and new commercial synthesis of sertraline HCl (use of green solvent) (iii) Use of biocatalyst to replace Cr based catalyst in the synthesis of LY 300164 (iv) Improved ecological footprint in the synthesis of Celecoxib (v) Quinaprin synthesis avoiding the use of potentially explosive hydroxybenzotriazole.
Green technologies in generic pharmaceutical industry: Current Vs greener method, ex; bromination (Reddy's lab).

10. FLOW CHEMISTRY (3+2) hours

Introduction: Batch vs flow operations, flow reactor, types of reactors. Meaning of residence time and molar flow rate.
Mass transfer: mixing rate vs reaction rate, Damkohler number, manipulation of Damkohler number: e.g., synthesis of Verubecestat.
Advantages of flow chemistry: Outpacing intramolecular reactions, e.g., Fries rearrangement.
Practical applications: Fischer esterification using in-line GC analysis.
Swern-Moffatt oxidation.
Handling hazardous reagents, ex; diazomethane, phosgene.
Limitations of flow chemistry

REFERENCES

1. Green chemistry-Theory and practice. Anastas P. C, Warner J. C., Oxford University Press, 1998.

2. Handbook of Research on Global Supply Chain Management, Ed; Brian Christiansen, Chapter 15, Sustainability-A Comprehensive Literature (IGI Global) 2016.
3. Organic Synthesis: Special Techniques, V. K. Ahluwalia and R. Aggarwal, Norosa, New Delhi, 2003.
4. Handbook of biodegradable polymers, ed; Andreas Lendlein and Adam Sisson, Wiley VCH, 2011.
5. Handbook of biodegradable polymers, ed Catia Bastioli (De Gruyter), 3rd edition, 2020.
6. Green chemistry: Environmentally friendly alternatives, R. Sanghi and M. M Srivastava, Norosa, New Delhi, 2003.
7. Green Chemistry-an introduction text, The Royal Society of Chemistry.
8. Green Chemistry in Pharmaceutical Industry, Peter J. Dunn, Andrew S. Wells and Michael T. Williams. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.
9. Supercritical Carbon Dioxide in Polymer Reaction Engineering, Kemmere, M. F., Meyer, T. (eds.) 2005.
10. Green synthesis interventions of pharmaceutical industries for sustainable development, Mohit Mishra, Mansi Sharma, Ragini Dubey, Pooja Kumari, Vikas Ranjan, Jaya Pandey. Current Research in sustainable Chemistry, 2021, 4, 100174.
11. Green process chemistry in the pharmaceutical industry, Berkeley W. Cue. Green Chemistry Letters and Reviews, 2009, 2, 193-211.
12. Flow Chemistry applications. Ed: Ferenc Darvas, Gyorgy Dorman, Volker Hessel and Steven V. Ley. 2nd edn. Walter de Gruyter GmbH and Co KG, 2014.
13. Organocatalysis. Ed: M. T. Reetz, B. List, S. Jaroch, H. Weinmann, 1st edn. Springer, 2007.
14. Christoph Grondal, Matthieu Jeanty and Dieter Enders. Organocatalytic cascade reactions as a new tool in total synthesis. Nature Chemistry, 2010, 2, 167-179.
15. Burstein C, Glorius F. Organocatalyzed conjugate umpolung of α, β-unsaturated aldehydes for the synthesis of γ-butyrolactones. Angew Chem Int Ed, 2004, 43, 6205–6208.
16. Berkessel A, Andreae MRM. Efficient catalytic methods for the Baeyer-Villiger oxidation and epoxidation with hydrogen peroxide. Tetrahedron Lett, 2001, 42, 2293–2295.
17. Berkessel A, Adrio JA. Dramatic acceleration of olefin epoxidation in fluorinated alcohols: activation of hydrogen peroxide by multiple H-bond networks. J Am Chem Soc, 2006, 128, 13412–13420.

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

LO1	Knowledge	Define organocatalyst, supported organocatalyst, sustainability, biodegradable polymers, supercritical fluid and solvent-free reaction, residence time, molar flow rate and Damkohler number List the types of PTC reactions, flow rectors, precursors for and generation of NHC, basic principles and challenges of sustainability, restrictions on one-pot reactions, the advantages and disadvantages of ultrasound and microwave methods, flow chemistry, use of polymer supports, biodegradable polymers from petroleum sources and renewable resources Recall the principles of green chemistry, PTC reactions, Swern-Moffatt reaction Draw the structures/partial structures of crown ethers, polymer supports, NHC, enamine and iminium ion, drug molecules.
LO2	Understand	Classify biodegradable polymers, one-pot reactions, PTC reactions, supported organocatalysts, solvents based on greenness factor, polymer supports based on solubility Explain mechanism of one pot reactions, models of sustainability and sustainability issues, draw backs of biodegradable polymers and their modification, different types of separation techniques in polymer supported synthesis, α-heteroatom functionalization, direct conjugate additions via enamine activation, transfer hydrogen reactions Distinguish between the types of mechanochemical methods, enamine and iminium ion organocatalysis, batch and flow reactors, crown ethers and CD
LO3	Apply	Calculate % atom economy and E-factor Examine the suitability of the conditions of a reaction to be a green reaction, effect of various parameters on selectivity of the product, conversion and on yield, mechanism of PTC based on the reaction conditions Illustrate the use of PS for oligosaccharide and peptide synthesis, Dieckmann condensation, role of organocatalyst in obtaining chemoselective product and highlight the green chemistry involved, the role of water as solvent under different conditions- under pressure enabling reactions at high temperature, case study of drug molecules. Apply flow chemistry in Fries rearrangement and Fischer

		esterification Relate variously substituted onium salts to efficiency of extraction
LO4	Analyze	Relate the various types of economy to one-pot reactions and the structure of the polymer support to the desired product Analyse the effect of base on the mechanism of PTC, influence of parameters on extraction by PTC and crown ethers, the effect of NHC on conjugate Umpulong addition to α, β-unsaturated aldehydes Case study-Correlate the selectivity of products to the parameters of coupling reactions. Identify the given molecules as electrophile and nucleophile Predict the suitability of convergent methods over linear methods in green synthesis of drug molecules
LO5	Evaluate	Predict the product distribution/ selectivity based on the ball milling parameters, the type of PTC reaction Assess the convergent synthesis of sildenafil citrate over linear strategy in obtaining clean product, the suitability of the PS based on the structure, synthesis and separation method Evaluate the suitability of organocatalyst over conventional catalyst in Aldol and Michael addition reaction
LO6	Create	Modify the method available for the synthesis of the PTC, PS-synthetic route for a given oligonucleotide, Dieckmann cyclisation product, Wittig's reaction and an organocatalyst for chemoselective reaction. Prepare an outlay of synthetic route for oseltamivir (case study) by one-pot reaction and modify the synthetic strategy based on the condition, selective epoxidation reaction using hydrogen bonding networks, crown ethers by alternate methods Compose a ring closure reaction for the synthesis of heterocyclic compound and a dehydrohalogenation reaction under PTC conditions.

QUESTION PAPER PATTERN-ESE

St. Joseph's University, Bengaluru-27
M.Sc. End Semester Examination
(2024-25 onwards)
ANALYTICAL / ORGANIC CHEMISTRY

Time: 2 hours **Max. Marks: 50**

Instructions

1. Question paper has three Parts. Answer all the Parts.
2. Write chemical equations and diagrams wherever necessary.

PART– A

Answer any **EIGHT** of the following TEN questions. Each question carries **TWO** marks. **(8 x 2 =16)**

PART– B

Answer any **TWO** of the following THREE questions. Each question carries **TWELVE** marks. **(2 x 12 = 24)**

PART– C

Answer any **TWO** of the following THREE questions. Each question carries **FIVE** marks. **(2 x 5= 10)**

Note: The questions must have the weightage of 25% portions from the mid semester exam portion and 75% weightage from the portion covered after mid semester examination.

MID-SEM EXAM PATTERN

St. Joseph's University, Bengaluru-27
M.Sc. Mid Semester Examination
(2024-27)
ANALYTICAL / ORGANIC CHEMISTRY

Time: 1 hour **Max. Marks: 25**

Instructions

1. Question paper has three Parts. All parts are compulsory.
2. Write chemical equations and diagrams wherever necessary.

PART– A

Answer any **FOUR** of the following SIX questions. Each question carries **TWO** marks.

(4 x 2=8)

PART– B

Answer any **ONE** of the following TWO questions. Each question carries **TWELVE** marks.

(1 x 12 = 12)

PART– C

Answer any **ONE** of the following TWO questions. Each question carries **FIVE** marks.

(1 x 5= 5)

EVALUATION PATTERN- PRACTICALS

Formative Assessment (Internal assessment) Practicals (35)	Continuous evaluation	25
	Viva voce	10
End semester practical examination (ESPE)		15
Total Marks		**50**