ST JOSEPH'S UNIVERSITY

BENGALURU - 27

SCHOOL OF CHEMICAL SCIENCES

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ORGANIC 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 of 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 CREDITS**	**TOTAL MARKS**
SEMESTER III				
THEORY				
Paper I	OCH9125: Organic Synthesis-I	4	4	60
Paper II	OCH9225: Organic Synthesis-II	4	4	60
Paper III	OCH9325: Chemistry of Heterocyclic Compounds, Biomolecules and Natural Products	3	3	45
Paper IV	OCH9425: Stereochemistry and Asymmetric synthesis	4	4	60
	PRACTICAL			
Paper I	OCH9P1: Separation and identification of organic compounds	4	1.5	50
Paper II	OCH9P2: Organic Synthesis - 1	4	1.5	50

	(one-stage and two-stage preparations)			
Paper III	OCH9P3: Organic Synthesis-II (advanced organic synthesis)	4	1.5	50
Paper IV	OCH9P4: Organic Synthesis-III (green methods of organic synthesis)	4	1.5	50
		TOTAL	**6**	**200**
SEMESTER IV				
Paper I	OCH0225: Medicinal Chemistry	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 number of credits: 26				
KEY WORDS: DE – Departmental 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 in a 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*** and molecular ions (H_2 to O_2), 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 the 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 4hours

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 = 15hrs

Resonance, field effects, hyperconjugation, steric effects and steric inhibition of resonance on reactivity.

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 = 17 hrs

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 pseudoasymmetric centres.

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

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).* ***Conformations of mono-substituted cyclohexanes***, 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 11hrs

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 hrs

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=11 hrs

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, J. Clayden, N. Greeves, S. Warren, 2nd Edn., 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, 6th Edn., P. Sykes, Pearson education limited, 1986.
4. Stereochemistry of Carbon Compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley and Sons, 1994.
5. Stereochemistry of Organic Compounds, D. Nasipuri, Wiley Eastern, New Delhi, 1991.
6. Advanced Organic Chemistry, Part A, 5th Edn., F. A. Carey and J. Sundberg, 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, and mechanisms 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; eigenvalue 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 **12hrs**

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 4hrs

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: At the end of the course, the student 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

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

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

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+1hrs

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 theory of the Raman effect, quantum theory of 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 Edn., F.A. Cotton, Wiley Eastern, 2009.
2. Introduction to Molecular Spectroscopy, C.N. Banwell, M. McCash, TMH Pub, 2010.
3. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill, 1988.
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill, 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, 2008.

Learning Outcomes: At the end of the course, the student 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 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. 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,2nd Edn., J. H.Kennnedy, Cengage Delmar Learning India Pvt.Ltd., 2011.
6. Quantitative chemical analysis, 10th Edn., D. C. Harris, W. H. Freeman and Company, 2019.
7. Vogel's Textbook of quantitative chemical analysis, 6thEdn.,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, 2ndEdn., F. Rouessac, A. Rouessac, John Wiley & Sons Ltd, 2007.

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

LO1	Remember	Differentiate the various radicals present in salt mixtures including rare cations.
LO2	Understand	Explain the concept of solubility product and common ion effect.
LO3	Apply	Perform analysis of cations and anions in a salt mixture samples.
LO4	Analyze	Perform analysis of salt mixture samples containing more number of cations and anions Practice strict safety protocols, understand the handling of hazardous chemicals.
LO5	Evaluate	Compare systematic analysis with spot tests.
LO6	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 hours per week	4
Total number of teaching hours 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- 1session

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 using 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 Outcomes: At the end of the course, the student should 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 sessions)
2. Saponification value of oil/fat. (1 sessions)
3. Estimation of glucose. (1 sessions)
4. Estimation of phenols by acylation method. (1 sessions)
5. Iodine value of oil/fat (1 sessions)
6. Estimation of glucose and sucrose in a mixture (1 sessions)
7. Estimation of acetone by Iodometry. (1 sessions)
8. Determination of amine salts by titration in aqueous solutions (1 sessions)
9. Estimation of nitro group. (1 sessions)
10. Estimation of nitrogen Kjeldhal's method. (1 sessions)
11. Estimation of carbonyl group by hydroxylamine-pyridine method. (1 sessions)
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 Organic Analysis, Clarke and Hayes 1964.

Learning Outcomes: At the end of the course, the student should 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**

Basic concepts of co-ordination chemistry. 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). ***MO energy level diagrams in tetrahedral complexes***.

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.

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

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+}).

5. 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***.

6. 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 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 parentheses and italics correspond to recall/review.

1. ADDITION REACTIONS **8+2 hours**

Addition to carbon-carbon multiple bonds: ***General mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity***; 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. ***Addition of Grignard reagents and organolithium reagents to carbonyl compounds***

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.

***Halogenation of aldehydes, ketones and acids, haloform reaction*.**

3. REARRANGEMENTS **14+1 hours**

Carbon to carbon migrations: ***Wagner-Meerwein, pinacol-pinacolone***, 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 rearrangemen.

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.

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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.
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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, ***derivation of equation for fraction of molecules occupying a given energy range***. Fermi-Dirac statistics: assumptions, ***derivation of equation for fraction of molecules occupying a given energy range***. 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. ***Application of statistical thermodynamics: equipartition theorem, heat capacity behavior of crystals.***

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, Nernst distribution 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 and forces 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.
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5. Principles of Physical Chemistry, B.R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishersco, 2017.
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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 overallformation 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 ofsystems, 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 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 and vibrational partition function. **Choose** the solvents in the increasing order of reaction rate between a pair of 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 the decomposition 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 tounderstand 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 pair of 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 after mixing 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/ko) 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 (^1J); two-bond couplings (^2J); three-bond couplings (^3J)-Karplus relationship. Long-range couplings (^4J-^nJ); 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.
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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.

High performance thin layer chromatography, forced flow planar chromatography. 2D TLC. Application of TLC.

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.

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.

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, 10th 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, 2nd 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, 10th Edition, Cengage Learning, 2022.
6. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 5th edition, Saunders College Publishing, International Limited, 1999.
7. Introduction to modern liquid chromatography, Lioyd R. Snyder, J J Kirkland, J W Dolan, 3rd Edn, Wiley Publication, 2010.
8. Principle and Techniques of Biochemistry and Molecular Biology, Walker Jon and Keith Wilson, 8th 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	PREPARATION AND CHARACTERIZATION- I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Organic synthesis, purification, characterization: (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 relevant 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 Edn., 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, 2nd Edn., 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: 6th Edn., K. Nakamoto, John Wiley & Sons, 2009.

Learning Outcomes: At the end of the 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. Preparation of benzanilide from benzophenone (2 sessions)

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

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

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

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

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

7. Preparation 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	OCH9125
Paper title	ORGANIC SYNTHESIS-I
Number of teaching hours per week	04
Total number of teaching hours per semester	60
Number of credits	04

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

1. IMPORTANT REACTIONS IN ORGANIC SYNTHESIS 7+1 hours

C-C bond formation: Henry, Peterson's olefination, Bamford-Stevens, McMurry coupling, Robinson Annulation, Stobbe reaction, Darzen's reaction, Horner-Wadsworth-Emmons, Shapiro reaction.
C-O bond formation: Stork-enamine synthesis, Acyloin condensation.
C-N bond formation: Barton reaction, Mannich reaction
Wittig reaction, Perkin reaction, Dieckmann condensation, Claisen ester condensation, Knoevenagel condensation.

2. OXIDATION-REDUCTION REACTIONS IN ORGANIC SYNTHESIS 12+1 hours

Applications of peroxides (hydrogen peroxide, *t*-butyl peroxide, dibenzoylperoxide), peracids (CF_3COOOH, m-CPBA) as oxidizing agents, HIO_4, DDQ, Selenium dioxide, Chromium (VI) and Manganese (VII) as oxidants. Dess-Martin oxidation, Sharpless asymmetric epoxidation and Oppanaeur oxidation.
Complex metal hydrides, diimide reduction, organoboranes, LDA, trimethylsilyl iodide, Woodward and Prevost reagent, NBS, Benkeser reduction, Wolf-Kishner reduction, Meerwin-Pondorff Verley reduction, Pummer, Willgredot, Corey-Bakshi-Shibata reaction and Tischenko reaction.
Applications of Ozone and Osmium tetroxide as oxidants, Birch and Clemmenson reduction.

3. ORGANOMETALLICS IN ORGANIC SYNTHESIS **7+1 hours**

Organolithium compounds - application in deprotonation of C-H bonds, ortho directing effect, addition to multiple bonds (anionic polymerization), lithium-halogen exchange, synthesis of organometallics (via transmetalation). Organomagnesium compounds (Grignard reagent), application in organic and organometallic synthesis, Sulfonium ylides in organic synthesis, application of organozinc compounds (ZnR_2) in Simmons-Smith reaction.

4. TRANSITION METAL COMPLEXES (HOMOGENEOUS CATALYSIS) IN ORGANIC SYNTHESIS **14+2 hours**

Catalytic cycle and key reaction steps in homogeneous catalysis-ligand dissociation, association, oxidative addition-reductive elimination, substrate coordination, insertion/de-insertion, transmetalation, nucleophilic attack on substrate.

Catalytic hydrogenation (catalytic cycle of Wilkinson Catalyst), Asymmetric hydrogenation including transfer hydrogenation (Noyori catalyst with mechanism). Hydroformylation reaction of alkenes.

Alkene metathesis reactions-mechanism, Schrock catalyst, Grubbs catalysts (I and II generation)

Metal catalyzed coupling reactions: Pd catalyzed cross-coupling reactions, mechanism of overall cross coupling reactions, effect of catalyst structure on cross coupling reactions (effect of chelation, effect of steric properties, ligand electronic properties), substrate scope, reaction conditions (catalytic precursors, phosphine and N-heterocyclic carbene ligands), Mizoroki-Heck reaction (catalytic cycle with examples), application of Suzuki, Negishi, Kumada, Hiyama, Stille reactions, Tsuji-Trost (mechanism) and Buchwald-Hartwig reactions (catalytic cycle with examples). Copper catalyzed C-C and C-heteroatom bond forming reactions: Ullmann type, Chan-Lam Coupling.

18- and 16-electron rules. Current trends in homogeneous catalysts.

5. C-H BOND ACTIVATION IN ORGANIC SYNTHESIS **4+1 hours**

Introduction: Importance of C-H activation, types of C-H bond activation, green chemistry involved in C-H activation.

Mechanism of different types of C-H activation: ***radical-mediated***, metal mediated (homolytic, heterolytic and σ-bond metathesis pathways). Example: Palladium catalyzed C-H bond activation reactions.

Chelation assisted functionalization of arenes

C-H bond activation of heteroaromatics, ***metal-catalyzed oxidation of C-H bond to C-N bond***.

6. HETEROGENEOUS CATALYSIS IN ORGANIC SYNTHESIS 4+1 hours

Introduction, difference between homogeneous and heterogeneous catalyst, characteristics of heterogeneous catalysts, active sites in catalysts

Types of heterogeneous catalysis with examples.

Heterogenising aspects of homogeneous transition metal complexes: Anchored catalyst-introduction, need and advantages, anchored Wilkinson's catalyst, immobilization of transition metal complex catalysts on inorganic supports, active sites, leaching mechanism.

7. INTRODUCTION TO ELECTRO-ORGANIC SYNTHESIS 4+1 hours

Introduction: ***Electrode potential, cell parameters, electrolyte, working electrode***, choice of solvents, supporting electrolytes. Cell design: Undivided, quasi-divided and divided cell. Modes of operation-Galvanostatic and potentiostatic.

Anodic oxidation: Kolbe reaction, non-Kolbe oxidation, Shono oxidation, selective C-H activation reactions (arylation).

Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins and arenes.

REFERENCES

1. Advanced Organic Chemistry. Part B: Reactions and Synthesis. F. A. Carey and R. J. Sundberg, 5th edition, Springer publishers, 2007.
2. Organic Synthesis, M. B. Smith, 4th Edition, Elsevier Inc. 2017.
3. Modern Methods of Organic Synthesis, W. Carruthers and L. Coldham, 4th Edition, Cambridge University Press, 2004.
4. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2012
5. Organotransition Metal chemistry, J. F. Hartwig, University Science Books, 2010.
6. Basic Organometallic Chemistry, A. J. Elias, B. D. Gupta, 2nd Edition, Universities Press, 2013.
7. Organometallics and Catalysis, M. Bochmann, Oxford University Press, 2015.
8. Catalysis, Editors: U. Hanefeld and L. Lefferts, Wiley-VCH Verlag GmbH & Co., 2018.
9. Organometallics, C. Elschenbroich, 3rd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2006.
10. The Organometallic Chemistry of Transition Metals, R. H. Crabtree, 6th Edition, John Wiley & Sons 2014.
11. Metal-Catalyzed Cross-Coupling Reactions and More, 2nd Edition. Editors: A. de Meijere, S Bräse, M Oestreich, Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2014.
12. C-H bond activation in organic synthesis. Editor: J. J. Li., CRC Press, 2017.

13. Applied Homogeneous Catalysis with Organometallic Compounds 3rd Edition, Editors: B. Cornils, W Hermann, M Beller and R Paciello, Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, 2018.
14. Organic electrochemistry, O. Hammerich and B. Speiser, 5th Edition, CRC Press, 2016.
15. Fundamentals and Applications of Organic Electrochemistry, T. Fuchigami, M. Atobe and S. Inagi, John Wiley & Sons 2015.
16. Modern Heterogeneous Catalysis, an Introduction by R. A. van Santen, 1st Edition, Wiley VCH, 2017.
17. Heterogeneous Catalysis in Organic Chemistry; V. S. Gerard, N. Ferenc, 1st Edition, Academic Press New York, 2006.
18. Introduction to Surface Chemistry and Catalysis, G. A. Somorjai, Wiley, New York, 1994.
19. Heterogeneous Catalysis for the Synthetic Chemist, R. L. Augustine, Dekker, New York, 1995.
20. Heterogeneous Catalysis, D. K. Chakrabarty, B. Viswanathan, New Age Science, 2009.

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

LO1	Knowledge	Recall various C-C, C-N and C-O bond formation reactions, types of C-H bond activation and organometallic compounds List ligand, metal compounds and complexes as catalysts.
LO2	Understand	Explain the mechanism and catalytic cycles of various C-C, C-N and C-O bond formation reactions, types of C-H activation, cell design and mode of operations in electro-organic synthesis. Differentiate between active catalyst and precatalyst.
LO3	Apply	Apply suitable reagents for oxidation/reduction reactions, catalysts for C-C, C-heteroatom bond forming reactions and C-H activations, strategies for heterogenization of homogeneous catalysts, anodic oxidation and cathodic reduction in organic synthesis. Predict the major products for a given set of conditions, reagents and catalysts for given transformations. Provide alternative reaction conditions, catalyst etc., for a given organic synthesis.
LO4	Analyze	Compare and contrast the oxidizing or reducing power of various oxidants or reductants in organic synthesis.

		Assess the regio-, stereo-selectivities for a given organic transformation.
LO5	Evaluate	Deduce plausible mechanisms for anodic oxidation and cathodic reduction by electrode under a given reactions condition like, suitable substrates, electrodes, electrolytes and solvent.
LO6	Create	Design synthesis of a complex organic molecules using chemical C-H activation /electrochemical method / organo - metallics complexes as catalysts.

Semester	III
Paper code	OCH 9225
Paper title	ORGANIC SYNTHESIS-II
Number of teaching hours per week	03
Number of teaching hours per semester	45
Number of Credits	03

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

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

1. RETROSYNTHESIS: THE DISCONNECTION APPROACH (28+2) hours

Basic principles; introduction to synthons and synthetic equivalents. **2 h**
Synthesis of aromatic compounds and order of events. One-group C-X and two-group C-X disconnections. Reversal of polarity. Cyclization reactions; amine synthesis. **12 h**
Protecting groups: protection of alcohols, carbonyl compounds, amines and carboxylic acids. One group C-C disconnections. ***Choosing disconnections and regioselectivity*** ***and chemo selectivity.*** Alkene synthesis: Use of acetylides and aliphatic nitro compounds in synthesis. Two group C-C disconnections: carbonyl compounds, Diels-Alder reactions; 1,3-, and 1,5-, difunctionalized compounds, α, β-unsaturated carbonyl compounds, condensations, Michael addition and Robinson annulation. Introduction to Ring synthesis: synthesis of 3,4,5,6 membered rings and saturated heterocycles**.** **12 h**
Convergent synthesis: Differences between convergent and linear synthesis. Advantages of convergent synthesis over linear synthesis. Convergent synthetic strategy for Ferruginol, α-Bisabolene and Lycorane. Failure of convergent synthesis with Multistriatin as example. Linear synthesis of Multistriatin.
Combination of linear and convergent synthesis; starting material and key aspects of reaction, industrial synthesis of α- and β-sinensals as examples**.** **4 h**

2. REVIEW ARTICLE BASED MODERN ASPECTS OF ORGANIC CHEMISTRY (11+4) hours

REFERENCES

1. Organic Synthesis: The Disconnection Approach by Stuart Warren, 2nd Edition, Wiley India, 2008.
2. Workbook for Organic Synthesis-The disconnection Approach, Stuart Warren, 2nd Edition, John Wiley, 2010.
3. Organic Synthesis by Christine Wills and Martin Wills, Oxford University Press, 2005.

4. Organic Synthesis-Design, Reagents, Reactions and Rearrangements, Jagadamba Singh and D. S. Yadav, Pragati Prakashan, 2007.
5. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, 3rd Edition, CRC press, 1993.
6. Advanced Organic Chemistry, Francis A. Carey and Richard J. Sundberg, Part A- Structure and Mechanisms, 5th Edition, Springer Science, 2007.
7. Advanced Organic Chemistry by Francis A. Carey and Richard J Sundberg, Part B- Reactions and Synthesis, 5th Edition, Springer Science, 2007.
8. Nonenzymatic Reactions in Natural Product Formation
Leah M. Bouthillette, Victor Aniebok, Dominic A. Colosimo, David Brumley, and John B. MacMillan, Chem. Rev., 2022, 122, 14815.
9. Amide Activation: An Emerging Tool for Chemoselective Synthesis Daniel Kaiser, Adriano Bauer, Miran Lemmerer and Nuno Maulide Chem. Soc. Rev., 2018, 47, 7899.
10. Glycoconjugates: Synthesis, Functional Studies and Therapeutic Developments
Sachin S. Shivatare, Vidya S. Shivatare, and Chi-Huey Wong, Chem. Rev., 2022, 122, 15603.
11. Making Chiral Salen Complexes Work with Oraganocatalysts, Yu-Chao Yuan, Mohamed Mellah, Emmanuelle Schulz and Olivier R. P. David, Chem. Rev., 2022, 122, 8841−8883.

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

LO1	Knowledge	Define terms involved in retrosynthesis, name the type of disconnections and write the synthons based on the disconnection List umpolung synthons, types of selectivity encountered in synthesis, protecting groups
LO2	Understand	Explain the order of events in the synthesis of organic compounds, classify the types of C-X and C-C disconnections and give examples for these Predict the synthons for a given synthesis Differentiate convergent and linear synthesis
LO3	Apply	Illustrate the use of acetylenes, nitro compounds in organic synthesis Demonstrate the use of protecting groups in synthesis Draw the sequence of reactions for convergent and linear synthesis of natural products
LO4	Analyze	Carry out RSA of the given compound and arrive at synthons and outline a possible synthesis Examine the correctness of the disconnections Identify the correct set of synthons for a target molecule Arrange the protecting groups in the order of stability under given

		conditions
LO5	Evaluate	Assess the suitability of the given RSA and synthesis Justify the chosen disconnection Evaluate the given synthetic strategy
LO6	Create	Develop a synthetic strategy for a given target molecule Improve the synthesis using RSA and predict the outcome of the reaction Develop a protecting group and method of deprotection for a functional group

Semester	III
Paper Code	OCH9325
Paper title	CHEMISTRY OF HETEROCYCLIC COMPOUNDS, BIOMOLECULES AND NATURAL PRODUCTS
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 underlined correspond to self-study.
2. Text within parenthesis and italics correspond to recall/review

1. HETEROCYCLIC CHEMISTRY **(19+2) hours**

Five-membered heterocycles with one heteroatom: pyrrole, furan and thiophene- aromaticity and reactivity order, resonance, synthesis and chemical reactivity.

Six- membered heterocycles with one heteroatom: basicity, synthesis and chemical reactions of quinoline, isoquinoline, indole.

Azoles: synthesis and chemical reactions of 1,2,3-triazole, 1,2,4-triazole and 1,3,4-oxadiazole.

Azines: diazines (pyridazine, pyrimidine, pyrazine) and triazines (1,2,3-triazine, 1,2,4-triazine & 1,3,5-triazine).

Benzo-fused heterocycles: synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles and benzothiazoles.

Three and four membered oxygen and nitrogen containing heterocycles- name and structure.

2. PEPTIDES AND PROTEINS **7 hours**

Synthesis of peptides: chemical and Merrifield synthesis. Introduction to proteins. Difference between peptides and proteins. Ramachandran plot, super secondary structures in proteins, intrinsically disordered proteins, protein conformational switches and its significance, post-translational modifications in proteins.

3. CARBOHYDRATES **(6+1) hours**

Sugar derivatives: amino sugars and uronic acids. Polysaccharides: homo polysaccharides- dextrans and dextrins, chitin and inulin; hetero polysaccharides- peptidoglycan, pectin and glycosaminoglycans. Glycoconjugates: proteoglycans and glycoproteins. Chiral recognition and role of sugar in biological recognition.

Classification, structure and general properties of carbohydrates

4. LIPIDS **(3+1) hours**

Structure and biological importance of acylglycerols, phospholipids, glycolipids and sphingolipids.

Definition, general functions, classification into simple, compound and derived lipids, nomenclature of fatty acids.

5. STEROIDS AND PROSTAGLANDINS **7 hours**

Steroids: Introduction, stereochemistry structure elucidation and biosynthesis of cholesterol. Cholesterol as a precursor for steroid hormones, Vitamin D and bile acids.

Prostaglandins: Introduction to eicosanoids, nomenclature, classification and biological role of prostaglandins. Biosynthesis of prostaglandins and thromboxanes. Structure elucidation and stereochemistry of PGE1. Synthesis of PGE2 by Corey's approach.

6. TERPENES **(8+1) hours**

Structural elucidation, biosynthesis and synthesis of α-pinene (an example of bicyclic monoterpene), farnesol (an example of acyclic sesquiterpene) and abietic acid (an example of tricyclic diterpene).

Carotenoids: Methods of isolation, structural relationship of α -, β- and γ- carotenes. Structure elucidation, biosynthesis and synthesis of β-Carotene. Conversion of β-carotene to Vitamin A.

Classification, nomenclature, occurrence, isolation of terpenes. Isoprene rule, stereochemistry of citral, limonene, menthol and borneols.

7. ALKALOIDS **(4+1) hours**

Structural elucidation, biosynthesis and synthesis of Quinine (an example of quinoline alkaloid) and Morphine (an example of opiate alkaloid).

Definition, nomenclature, occurrence and classification of alkaloids.

REFERENCES

1. S. P. Bhutani. Organic Chemistry: Selected topics. Ane Books, 2008.
2. J. A. Joule, K. Mills, G. F. Smith. Heterocyclic Chemistry. 5th Edition, John Wiley and sons Ltd., 2010.

3. Raj. K. Bansal. Heterocyclic Chemistry. 5th Edition, New Age International publishers, 2017.
4. S. P. Bhutani. Chemistry of Biomolecules: Selected topics, Ane Books, 2008.
5. Biochemistry, Debajyoti Das, 14th Edition , Academic Publishers, 2010.
6. Fundamentals of Biochemistry, J.L Jain, S Jain and N. Jain S, 7th Edition, Chand Publications, 2016.
7. Principles of Biochemistry, Lehninger, 8th Edition, Macmillan Higher Education, 2021.
8. Biochemistry, L. Stryer, 9th Edition, WH Freeman, 2019.
9. I. L. Finar, Organic Chemistry, Vol II, Stereochemistry and the Chemistry of Natural Products Fifth Edition, Pearson 2009.
10. O. P. Aggarwal, Organic Chemistry Natural Products, Volume II, 38th Edition, Krishna Prakashan Media Pvt. Ltd., 2020.
11. Organic Chemistry of Natural products Vol I and II by Gurudeep R. Chatwal, editor: M. Arora, Himalaya publishing House, New Delhi, 2015.
12. Medicinal Natural Products, P. M. Dewick, 3rd Edition, John Wiley, 2011.

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

LO1	Remember	Recall the name and structures of 5-membered and 6-membered heterocyclic compounds, alkaloids, terpenes, steroids, prostaglandins and biomolecules Write the order of aromaticity and chemical reactivity of heterocyclic compounds and their resonance structures Draw the structural unit of amino acids and peptides. List protecting and deprotecting groups used for C-and N-terminal amino acids
LO2	Understand	Explain the chemical reactivity of heterocyclic compounds towards electrophilic and nucleophilic substitution, oxidation and reduction, Diels-Alder reaction and C-C coupling reaction, discuss the different methods of synthesis of 5- and 6-membered heterocyclic compounds, synthesis of peptides using solution phase and Merrifield resin strategy Describe structural elucidation, biosynthesis and synthesis of alkaloids, terpenes, steroids and prostaglandins, summarize the structural features and biological significance of biomolecules
LO3	Apply	Compare the basicity and reactivity towards substitutions reactions among 5-membered and 6-membered heterocycles having one or more hetero atoms, the stability of isomers of benzo-fused

		heterocycles Use several chemical reactions and spectroscopic techniques to identify a given terpene/ alkaloid/ prostaglandin/ steroid Determine the possible structural characteristics of a given biomolecule
LO4	Analyze	Distinguish between pyrrole, furan and thiophene; quinoline and isoquinoline; diazine and triazine based on their chemical reactivity, solid-phase and solution-phase synthesis of peptides Identify the product formed under given reaction conditions Classify and identify the given terpene/ alkaloid/ prostaglandin based on the evidence provided
LO5	Evaluate	Select the electron-rich and electron-deficient moieties among the given heterocyclic compounds Predict the structure of product formed in the given organic reaction. Summarize the role of substituent present in the molecule in determining the reactivity of molecule Justify the role of protecting and deprotecting groups in peptide synthesis Verify the structure of the given alkaloid/ terpene/ steroid/ prostaglandin using the steps of structural elucidation Examine how the structural features of biomolecules play an important role in their properties and biological function
LO6	Create	Compose a method for the synthesis of heterocyclic compound using the precursors provided Outline a method for the synthesis of heterocyclic molecule having substitution at a specific position Construct a synthetic strategy for the peptide using given sequence of amino acids Recognize the alkaloid/ terpene/ steroid/ prostaglandin provided the evidence of structural elucidation, precursors involved in the synthesis of given heterocyclic compound Determine the structure of the biomolecule from a set of information from chemical reactions

Semester	III
Paper code	OCH9425
Paper title	STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS
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 underlined correspond to self-study.
2. Text within parentheses and italics correspond to recall/review.

1. STEREOCHEMISTRY OF UNSATURATED ACYCLIC, FUSED, BRIDGED AND CAGED SYSTEMS **12+2 hours**

(*Stereochemistry of fused rings and bridged rings*).

Synthesis and stereochemistry of fused, bridged and caged systems: paddlanes and propellanes; catenanes, rotaxanes, knots, and Möbius strips; cubane, tetrahedrane, dodecahedrane, adamantane and buckminsterfullerene. ***Applications of molecules having bridged and caged systems.***

Conformations of unsaturated acyclic compounds such as carbonyl compounds, conjugated systems, etc. and ***miscellaneous compounds (alcohol, ether, peroxide, etc.).***

2. EFFECT OF CONFORMATION ON REACTIVITY **7+1 hours**

Diastereomer equilibria in acyclic systems.

Conformation and reactivity: the Winstein-Holness equation and the Curtin-Hammett Principle: Derivations and applications in organic synthesis.

3. ASYMMETRIC SYNTHESIS **14+2 hours**

'Enantiomeric excess' (*ee*) and methods of determination of '*ee*'. Stereoselectivity: classification, terminology and principle. Asymmetric synthesis and asymmetric induction. Double diastereoselection and double asymmetric induction.

Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4-asymmetric induction: Cram, ***Felkin-Ahn,*** Prelog models). Asymmetric aldol condensation, Zimmerman-Traxler model. Addition of allylmetal and allylboranes to carbonyl group.

Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, exo-endo selection), catalytic hydrogenation (haptophilic stereocontrol), alkylation (α-alkylation of (*S*)-proline), diastereoselective oxidations, enantioselection of OsO_4 dihydroxylation using chiral diamines, stereoselective cyclization of polyenes (biomimetic synthesis of progesterone).

Enantioselective synthesis: Reduction with chiral hydride donors [(*S*)-PBMgCl, (-)-iBOAlCl_2, alpineborane, (*S*)-BINAL-H, ***(R,R)-DIOP, (S,S)-CHIRAPHOS***].

Enantioselective alkylation of ketones via hydrazones (SAMP, RAMP). Enantioselective alkylation with chiral PTC. ***Enantioselective Michael addition. Enantioselective intramolecular aldol condensation and Robinson annulation***. Use of (+)- and (–)- DET in Sharpless asymmetric epoxidation. Asymmetric amplification.

Polymer-bound chiral catalysts in asymmetric induction.

4. CHIRAL RESOLUTION TECHNIQUES 7+1 hours

Separation of enantiomers via crystallization (conglomerates); chemical separation of enantiomers via diastereomers: introduction to resolving agents, resolving agents for a few functional groups (acids, lactones, bases, aldehydes, ketones and amino acids).

Diastereomers: Asymmetric transformations, general methods of separation, chromatographic resolution.

Enantiomeric enrichment as a resolution strategy in nonracemic samples.

Large scale resolution: diastereomer mediated resolution, resolution by preferential crystallization, kinetic resolution, enzymatic resolution.

chiral chromatography for enantiomeric resolution

5. METHODS TO DETERMINE CONFIGURATION 12 +2 hours

Bijvoet method-anomalous X-ray scattering, crystals as probes for assigning configuration, chemical correlation, study of quasi-racemates using melting point curves, spectroscopic methods such as CD, ORD, and NMR. Determination of absolute configuration by NMR: Chiral anisotropic reagents.

Chiroptical properties: optical activity, anisotropic refraction: theory, optical rotatory dispersion (ORD). Circular dichroism (CD), anisotropic absorption.

Applications of ORD and CD: Determination of configuration and conformation (theory); classification of chromophores; sector and helicity rules: α-axial haloketone rule, Octant rule, Benzene quadrant rule, Snatzke's Benzene sector rule, Lowe's rule for allenes; exciton chirality rule or dibenzoate chirality rule. Correlation of Optical rotation and group polarizability: Brewster's rule. ***Effect of solvent polarity on CD of (-)-menthone.***

Other applications: induced ORD and CD; fluorescence detected circular dichroism; circular dichroism of chiral polymers. Vibration optical activity. Circular polarization of emission; anisotropic emission.

REFERENCES

1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley and Sons, 2016.
2. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri,5th Edition., New Age International Publishers, 2022.
3. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, 11th Edition., New Age International Publishers, 2022.
4. Organic chemistry Volume 2: Stereochemistry and the Chemistry of Natural products, I. L. Finar, 5th Edition, Pearson Education India, 2002.
5. Circular Dichroism: Principles and Applications, N. Berova, K. Nakanishi, R. W. Woody, 2nd Edition., John Wiley & Sons Inc., 2000.
6. Chiroptical spectroscopy: Fundamentals and applications, 1st Edition., Prasad L. Polavarapu, CRC Press, Taylor & Francis Group, 2017.
7. Modern NMR Approaches to the Structure Elucidation of Natural Products, Volume 2, 1st Edition, Antony Williams, D. Rovnyak, G. Martin, Royal Society of Chemistry, 2016.

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

LO1	Knowledge	Identify examples of cage compounds from various chemical classes and common types of molecular conformations Describe mechanically interlocked molecules Recall the basics of stereochemistry and terminologies such as enantiomer, enantiomeric excess, chirality, prochiral centre and conformers. List the principles behind resolution methods used in separating racemic mixtures
LO2	Understand	Distinguish cage compounds from other types of molecules. Interpret the role of cage compounds in various chemical reactions or applications Describe how intermolecular forces affect molecular conformation. Explain the significance of cage compounds in organic chemistry, the reasons for special characteristics shown by cage molecules; the relationship between molecular conformation and reactivity in chemical reactions and the significance of resolution in separating enantiomers; asymmetric synthesis, partial asymmetric synthesis, principle of stereoselectivity, asymmetric induction, asymmetric

		amplification and chiroptical properties; the concepts and the stereochemical aspects of important reactions used in asymmetric synthesis Discuss various methods to determine relative and absolute configuration such as anomalous XRD, chemical correlation, preparation of quasi racemates, NMR and chiroptical properties
LO3	Apply	Illustrate different conformations of simple molecules like ethene, butene, etc. with diagrams Employ resolution techniques to purify chiral compounds in laboratory settings. Predict the stereochemistry of products in asymmetric synthesis based on various models; the ORD and CD curves of various types of molecules using empirical and semi-empirical theories Determine the stereochemical outcomes of organic reactions where multiple stereocentres are formed resulting in racemates, diastereomers etc. Examine the observed reactivity patterns in organic reactions with conformational considerations,
LO4	Analyze	Critically assess the potential applications of cage compounds in different fields Compare and contrast different types of cage compounds regarding their structures. Break down the mechanisms of chemical reactions based on the conformational changes involved Demonstrate the use of molecular modeling software to analyze molecular conformations and predict reactivity; the use of analytical techniques such as chiral chromatography in enantiomeric resolution Explore the stereochemical aspects of asymmetric synthesis involving simple molecules and use this information to predict the stereochemistry in the case of natural products
LO5	Evaluate	Interpret the influence of conformational effects on reaction rates and selectivity Compare and contrast the reactivity of molecules in different conformations; different resolution methods in terms of their advantages, limitations, and applicability Judge the suitability of specific cage compounds for particular applications based on their properties; the effectiveness of different strategies for controlling molecular conformation in organic

		synthesis; efficiency of resolution techniques in achieving high enantiomeric purity Recommend suitable chiral reagents to prepare a specific target molecule Evaluate different empirical and semi-empirical methods to predict signs of cotton effect curves to determine absolute configuration Assess the impact of conformational flexibility on the biological activity of drugs or biomolecules; the reliability of computational methods used in conformational analysis; the role of resolution in the development of pharmaceuticals and other chiral compounds
LO6	Create	Design novel cage compounds with specific structural features or properties; a new molecular machine for new chemical reaction; experiments to investigate the conformational preferences of specific molecules; experiments to optimize resolution conditions for a particular racemic mixture. Develop innovative strategies for the synthesis or modification of existing cage compounds and for modifying molecular structures to favor certain conformations for enhanced reactivity; novel resolution methods or modifications to existing techniques to improve efficiency or selectivity. Propose hypotheses regarding the influence of conformational changes on reaction mechanisms in novel chemical systems Plan a synthetic protocol to perform an asymmetric synthesis with better stereo selection Prepare strategies for integrating resolution processes into synthetic routes for chiral molecule synthesis

PRACTICALS

Semester	III
Paper Code	OCH 9P1
Paper Title	SEPARATION AND IDENTIFICATION OF ORGANIC COMPOUNDS
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

This practical course involves purification and analysis of a mixture of organic compounds. The components of the given mixture would be purified by recrystallization, solubility and distillation techniques, thin layer chromatography (TLC), column chromatography, high performance liquid chromatography (HPLC) followed by spectroscopic characterization. Application of advanced qualitative analysis: Preparation and characterization of organic compounds having *o*- and *p*- isomers (separation of isomers from crude products)

(11 sessions)

1. Purification of mixture of organic compounds by recrystallisation. (1 Session)
2. Identification and separation of mixture of organic compounds using TLC. (1 Session)
3. Separation of mixture of organic liquid compounds using distillation. (1 Session)
4. Separation of mixture of organic compounds using column chromatography. (1 Session)
5. Separation of mixture of organic compounds using HPLC. (1 Session)
6. Separation of mixture of organic compounds using solubility techniques and their structure elucidation using FT-IR and UV-vis spectroscopic techniques. (1 Session)
7. Separation of mixture of organic liquid compounds using distillation and their characterization using spectroscopic techniques. (1 Session)
8. Separation of mixture of organic compounds using column chromatography and their structural characterization using spectroscopic techniques. (1 Session)
9. Optical rotation of glucose and fructose using polarimeter. (1 Session)
10. Synthesis of an organic compound giving isomers/ Nitration of chlorobenzene to give mixture of *o*- and *p*-nitrochlorobenzene. (1 Session)

11. Identification of isomers of synthesized organic compound using TLC, purification using column chromatography and structural characterization using spectroscopic techniques. (2 Sessions)

REFERENCES

1. 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.
2. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd., 2018.
3. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, 2nd edition reprinted, New Central Book Agency (P) Ltd., 2018.

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

LO1	Knowledge	Recall the basic principle of recrystallisation, chromatography and distillation techniques, the terminology used in different chromatographic techniques Recall the basic instrumentation of UV-visible, FTIR, HPLC and polarimeter techniques
LO2	Understand	Explain the underlying principles of recrystallization, including solubility, saturation and crystal formation. Understand the importance of selecting an appropriate solvent and controlling temperature for effective recrystallization Describe the fundamental principles of polarimeter and different chromatographic techniques Use TLC to separate and identify components in complex mixtures, interpreting chromatograms to determine Rf values and relative polarities
LO3	Apply	Apply knowledge of recrystallization, solubility and distillation techniques to purify a mixture of organic compounds Apply knowledge of TLC principles to plan and execute TLC experiments, including selecting appropriate stationary phases, mobile phases, and visualization techniques Separate the mixture of organic compounds using TLC, HPLC and column chromatography Synthesize an organic compound and purify it using separation techniques

LO4	Analyze	Compare and contrast the properties of the purified compound before and after recrystallization Analyze HPLC chromatograms to interpret retention times, peak shapes and peak areas, identifying and quantifying analytes in complex mixtures
LO5	Evaluate	Evaluate the efficiency of different solvent systems and recrystallization methods, for purifying mixture of organic compounds Assess the loading of column based on TLC chromatogram of mixture of organic compound Formulate the results obtained by HPLC and polarimeter experiments
LO6	Create	Develop alternative approaches to traditional recrystallisation methods Design a column setup to separate any unknown mixture of compounds Data analysis of HPLC of any unknown mixture of compounds

Semester	III
Paper Code	OCH 9P2
Paper Title	PRACTICAL: ORGANIC SYNTHESIS- I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	1.5

This practical course involves single-step and two-step organic synthesis, characterization of the products through relatively simple techniques like thin layer chromatography and melting point determination. It also involves UV/IR spectral analysis and determination of percentage purity of the products by HPLC.

Organic synthesis, purification, characterization: (11 sessions)

1. Synthesis of adipic acid from cyclohexanol. (1 Session)
2. Synthesis of tetrahydrocarbazole from cyclohexanone and phenylhydrazine by Fischer indole synthesis. (1 Session)
3. Synthesis of Anthranilic acid starting from phthalic anhydride and urea (Hofmann rearrangement). (2 Sessions)
4. Synthesis of 2,5-hydroxyacetophenone starting from resorcinol and acetic acid (Fries rearrangement). (2 Sessions)
5. Synthesis of Benzilic acid starting from benzoin (Benzilic acid rearrangement). (2 Sessions)
6. Synthesis of polyhaloarene (1-iodo-2,4,6-tribromoaniline) starting from aniline. (2 Sessions)
7. Any other experiments/Viva (1 Session)

REFERENCES

1. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical, 1999.

2. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.

3. An Advanced course in Practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, 2nd Edition reprinted, New Central Book Agency (P) Ltd, 2018.

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

LO1	Knowledge	Recall various named reactions in organic transformations. Explain The multi-step synthesis of organic compounds.
LO2	Understand	Describe the mechanisms of various named reactions.

LO3	Apply	Select various catalysts and reagents in the preparation of organic compounds. Identify suitable reaction conditions in the preparation of organic compounds. Calculate the theoretical/percentage yields of compounds.
LO4	Analyze	Compare the various synthetic methods for an organic compound. Characterize the synthesized organic compounds using various spectral and chromatographic techniques.
LO5	Evaluate	Predict the spectral pattern for related compounds.
LO6	Create	Design synthetic routes for structurally related compounds.

Semester	III
Paper code	OCH 9P3
Paper title	PRACTICAL: ORGANIC SYNTHESIS-II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

This practical course involves slightly advanced organic synthesis meant to train students for higher academic/ industrial research, purification of the synthesized compounds, characterizations through simple techniques like thin layer chromatography and melting point analysis, and advanced instrumental characterization of the purified compounds. It also includes the spectral analysis of the compounds.

Organic Synthesis, purification, characterization: 11 Sessions

1. Preparation of dry solvents (1 session)
2. Protection and selective deprotection of functional groups (2 sessions)
3. Azidation using crown ethers (selective protection of primary alcohol) (2 sessions)
4. Wittig reaction (2 sessions)
5. Reduction of ester to alcohol using metal hydride (1 session)
6. Dicyclohexylcarbodiimide (DCC) mediated coupling reaction (1 session)
7. Grignard reaction (2 sessions)
8. Any other related experiments/RBPT (1 session)

REFERENCES

1. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.
2. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, 2nd Edition reprinted, New Central Book Agency (P) Ltd, 2018.

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

LO1	Knowledge	Recall various named reactions for organic transformations, organic chemistry principles and terminologies used in laboratory experiments. Memorize safety protocols and procedures for handling organic chemicals and equipment.
LO2	Understand	Describe the mechanisms of various organic reactions. Explain the fundamental concepts behind organic reactions such as reactivity trends Learn the technique of setting up reactions under anhydrous conditions and to prepare dry organic solvent. Interpret the spectral and chromatographic data of synthesized organic compounds
LO3	Apply	Apply various protection and de-protection strategies to obtain target organic molecule, spectroscopic methods (e.g., NMR, IR) to identify unknown organic compound Identify suitable reaction conditions to prepare air and moisture sensitive organic compounds Perform various organic synthesis techniques, including extraction, distillation, and chromatography, to isolate and purify organic compounds
LO4	Analyse	Analyse the results of organic reactions to determine the efficiency of the synthesis and the purity of the products Evaluate the reliability of experimental procedures and troubleshoot any issues encountered during organic synthesis
LO5	Evaluate	Evaluate experimental designs and propose improvements to optimize reaction conditions and increase yields. Assess the safety precautions taken during laboratory experiments and suggest enhancements to minimize risks
LO6	Create	Design new organic synthesis routes for the preparation of specific target molecules

Semester	III
Paper code	OCH 9P4
Paper title	PRACTICAL: ORGANIC SYNTHESIS-III
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	1.5

Organic Synthesis, purification, characterization (11 sessions)

This practical course involves comparatively greener methods of organic synthesis meant to train students for higher academic/ industrial research, purification of the synthesized compounds, characterizations through simple techniques like thin layer chromatography and melting point analysis, and advanced instrumental characterization of the purified compounds. It also includes the spectral analysis of the compounds.

Organic Synthesis, purification, characterization 11 sessions

1. Conversion of Benzhydrol to Benzophenone by different oxidation reactions and to assess the green chemistry index. (2 sessions)
2. Solvent-free reductive amination using mortar and pestle (2 sessions)
3. Proline catalyzed reaction in water (2 sessions)
4. Suzuki coupling in pure water (2 sessions)
5. 1,4-Cyclohexadiene with Pd/C as a rapid, safe transfer hydrogenation system with microwave heating. (1 session)
6. Microwave assisted nitration of phenol using copper nitrate. (1 session)
7. Photoxidation of alcohol with heterogeneous photocatalysts in the UV range (1 session)
8. Evaluation of the Photocatalytic degradation of Benzoquinone/2-chlorophenol in the aqueous phase using ZnO and TiO_2 Photocatalysts. (1 session)
9. Synthesis and Evaluation of biodiesel from waste vegetable oil (2 sessions)
10. Any other relevant experiments (1 session)

REFERENCES

1. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.
2. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, 2nd Edition reprinted New Central Book Agency (P) Ltd, 2018.

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

LO1	Knowledge	Recall the key principles of green chemistry, including minimizing hazardous substances and relevant organic chemistry reactions.
LO2	Understand	Explain whether the reactions are in accordance with the green chemistry principles Interpret spectral data for the product obtained in the organic reactions
LO3	Apply	Identify suitable reaction conditions for the preparation of organic compounds under green method; spectroscopic/chromatographic methods to estimate the concentration of unknown organic compound
LO4	Analyse	Assess different green methods for the synthesis of an organic compounds in terms of yield and green chemistry aspect.
LO5	Evaluate	Compare the different green chemistry methods of synthesis a particular compound on the basis of cost, energy, yield and green aspects and identify the best method.
LO6	Create	Design safer chemical reactions and processes, and utilizing renewable resources for the synthesis of any biologically important compound Propose solutions for a real-world scenario using green chemistry principle.

Semester	IV
Paper Code	OCH 0225
Paper Title	MEDICINAL CHEMISTRY
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. MOLECULAR ASPECTS OF DRUG ACTION (10 + 2) hours

Drug, API, drug additives (brief account of classification and meaning of different additives), Difference between drugs and medicines. Drug targets, receptors, receptor types, drug-receptor interaction (forces involved), agonist, antagonist, partial agonist (dose response curves), drug synergism, drug resistance, physicochemical factors influencing drug action, pharmacokinetics, pharmacodynamics, isosterism and bioisosterism, theories of drug – receptor interaction. Assay of drugs: Chemical assay, biological assay, immunological assay, ***LD_{50}, ED_{50}, IC_{50}, ID50 and EC_{50}. Metal ion toxicity and detoxification - chelation therapy***

2. CLASSIFICATION OF DRUGS BASED ON THERAPEUTICACTION (24+4) hours

Antibiotics: Introduction, targets of antibiotics action, classification of antibiotics, mechanism of action of penicillin, cephalosporin, β-lactamase inhibitors, tetracyclines, aminoglycoside and macrolides. Synthesis of penicillin.

Antivirals: Neuraminidase inhibitors (oseltamivir phosphate as an example), inhibitors of viral replication (acyclovir as an example), reverse transcriptase inhibitors (zidovudine and abacavir as examples). Synthesis of acyclovir.

Analgesics, antipyretics and anti-inflammatory Drugs: mechanism of inflammation, ***classification and mechanism of action of NSAID*** (aspirin, paracetamol and ibuprofen as examples). ***Synthesis of ibuprofen***.

Antihistamines: Mode of action of H1 and H2 antihistamines (chlorpheniramine, cetirizine and ranitidine as examples).

Antidiabetics: types of diabetics, types of drugs used for the treatment and their mode of action (sulfonylureas, α-glucosidase inhibitors, biguanides, dipeptidyl peptidase-4 (DPP-4) inhibitors,

Glucagon-like peptide-1 receptor agonists (GLP-1 receptor agonists), meglitinides, sodium-glucose transporter (SGLT) 2 inhibitors, sulfonylureas, thiazolidinediones). Synthesis of metformin.

Cardiovascular drugs: cardiovascular diseases, different classes of drugs acting on the cardiovascular system such as antianginal drugs, antiarrhythmic agents and antihypertensive agents.

Anti-neoplastic agents: Introduction, drug classes: alkylating agents- organoplatinum compounds, antimetabolites - purine, pyrimidine and folate drugs, antibiotics- actinomycins and anthracyclins, kinase inhibitors, natural products- mitotic inhibitors.

Central Nervous System (CNS) drugs: CNS depressants- anxiolytics, sedatives, hypnotics, antipsychotics. CNS stimulants- anti-depressants.

3. STAGES OF DRUG DISCOVERY AND DRUG DEVELOPMENT (11 + 1) hours

Procedure followed in drug design: drug discovery with and without a lead. Lead discovery.

Lead modification: Drug design and development, ADME, identification of active part: pharmacophore, functional group modification, structure-activity relationship (SAR). Structure modification to increase potency and the therapeutic index: homologation, chain branching, ring-chain transformation, bioisosteric structural modification to increase oral bioactivity (electronic effect, the Hammet equation & lipophilicity effect), peptidomimetics, Combinatorial chemistry.

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.

Clinical trials: Phase I, Phase II and Phase III trials.

4. PRODRUGS AND SOFT DRUGS (7 + 1) hours

Prodrugs as drug delivery systems: Utility of prodrugs, types of prodrugs; carrier-linked prodrugs: carrier linkages for various functional groups. ***Soft drugs: concept & properties***.

REFERENCES

1. An introduction to medicinal chemistry, G. L. Patrick, 5th edition, Oxford Publishers, 2013.
2. Burger's medicinal chemistry and drug discovery and development, Ed. D. J. Abraham and D. P. Rotella, 7th edition, Wiley-Blackwell Publishers, 2010.
3. The organic chemistry of drug synthesis, D. Lednicer, Vol. 6, Wiley-Blackwell Publishers, 1998.
4. The organic chemistry of drug design and drug action, R. B. Silverman and M. W. Holladay, 3rd edition, Academic Press, 2014.

5. Textbook of organic medicinal and pharmaceutical chemistry, C. O. Wilson, J. M. Beale and J. H. Block Wilson and Gisvold's, 12th edition, Published by Lipincott William & Willkins, 2011.

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

LO1	Knowledge	Describe the basic principles of medicinal chemistry; the different stages of drug development List the drugs based on pharmacological action Review the composition of different drugs and their side effects Recall the fundamental principles of drug design, including concepts such as pharmacophores, drug-receptor interactions, and structure-activity relationships (SAR); targets of antibiotic and antiviral drug's action and their significance in combating infections
LO2	Understand	Explain the importance and significance of drug absorption, distribution, metabolism pathways and excretion Relate the knowledge of pharmacokinetics and pharmacodynamics of a drug to their pharmacological activity, mode of action & adverse effect Narrate the principles of prodrug design & its application Explain the principles underlying the mechanism of action of antibiotics, antivirals, analgesics, anti-neoplastic agents, CNS drugs and cardiovascular drugs; the importance of specific drugs in treatment of bacterial infections, viral infections, pain, inflammation, cancer, neurological disorders and cardiovascular diseases; the synthesis of key drugs such as penicillin, acyclovir, and ibuprofen and their importance in pharmaceuticals Classify the structure-activity relationships of antibiotics, antivirals, analgesics, anti-neoplastic agents, CNS drugs, and cardiovascular drugs to predict their therapeutic uses and potential side effects
LO3	Apply	Utilize medicinal chemistry principles to design and optimize novel drug candidates, leveraging insights to enhance their efficacy and safety profiles Employ understanding of CNS drug mechanisms to evaluate their therapeutic potential in addressing neurological and psychiatric disorders; knowledge of cardiovascular drug mechanisms to examine their efficacy in managing cardiovascular diseases, applying discernment to determine their effectiveness. Implement prodrug principles to devise innovative drug delivery systems for improved therapeutic outcomes, applying creative strategies to enhance drug efficacy and patient outcomes
LO4	Analyze	Examine the molecular mechanisms of action of existing drugs and

		their potential for therapeutic efficacy and adverse effects Analyze structure-activity relationships and experimental data from biochemical and pharmacological studies Compare the efficacy of different drugs for same target
LO5	Evaluate	Assess the ethical, societal, and economic implications of drug development and use Evaluate the different drugs considering drug affordability, accessibility, and the balance between therapeutic benefits and risks; the effectiveness, safety profile and adverse effects of antibiotics, antivirals, analgesics, anti-neoplastic agents, CNS drugs, and cardiovascular drugs in clinical practice
LO6	Create	Modify the existing drugs considering factors such as potency, selectivity, pharmacokinetics, and safety profiles, using computational and experimental techniques Integrate knowledge from medicinal chemistry with insights from pharmacology, biochemistry, and other relevant disciplines to new drug development Design innovative strategies for addressing unmet medical needs through the development of new drugs or drug delivery systems Propose experiments to investigate the mechanism of action and efficacy of novel antibiotics, antivirals, analgesics, anti-neoplastic agents, CNS drugs, and cardiovascular drugs

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 hours**

Importance of solids in technological applications, solids as materials.

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***: general structural features, classification, intercalation and deintercalation***. 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 ***metal organic frameworks. Macroporous solids: Methods of preparation, properties and applications of opals and inverse opals***.

2. 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., 1997.
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. Chemistry of Nanomaterials, C.N.R Rao, Wiley VCH 2007.
6. Clemens Bruda, Chem. Rev. 2005, 105, 1025.
7. Vincent M Rotello, Nano Today, Vol 2,Number 3, June 2007.
8. Buddy Ratner, Allan S Hoffmann, Jack E Lemons, Frederick JSchoen, B.D. Ratner, Academic Press, 2004.
9. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Guozhong Cao, Imperial College Press, 2004.
10. Hybrid Nanocomposites for Nanotechnology: Electronic, Optical, Magnetic and Biomedical Applications, Lhadi Merhari, Springer Publications, 2009.

Learning outcomes: After the course completion, 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.

Diels-Alder reaction and oxidation of alcohols.

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.

Semester	IV
Paper code	CHDE 0425
Paper title	Dept. elective: FORENSIC 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. INTRODUCTION TO FORENSIC SCIENCE 11+ 2 hours

Definition, historical aspects, scope, code of conduct of forensic science. Crime Scene-types-indoor and outdoor. Securing and isolating the crime scene. Crime scene search methods.

Case study - Amanda Knox: A Flawed Case of Murder

Legal aspects of crime- Role of Investigator.

Case study - Dr. Coppolino's Deadly House Calls

Classification of crime scene evidence – physical and trace evidence. Collection, labeling, sealing of evidence.

Case study - Bruce McArthur: A Mountain of Physical Evidence.

Criminal Profiling -Profile of victim and culprit, its role in crime investigation, Lie detection (Polygraphy), Narco analysis, Brain mapping.

2. FINGERPRINTS 9 hours

Introduction- Basics of fingerprinting, Types of fingerprints. Fingerprint patterns. Development of Fingerprints- Latent prints. Latent fingerprints' detection by physical and chemical techniques.

Case study - Killer Twin: Ronald and Donald Smith

Case study - The Mayfield Affair

3. FORENSIC TOXICOLOGY 8 hours

Significance of toxicological findings. Techniques used in toxicology. Toxicological analysis – detection alcohol in blood sample, chemical intoxication tests - breath testing for alcohol. Human performance toxicology.

Case study-Accidental overdose: The Tragedy of Michael Jackson and Mac Miller.

4. ANALYTICAL METHODS IN FORENSIC CHEMISTRY 19+1 hours

Sample preparation for chromatographic and spectroscopic techniques. Chromatographic methods - forensic applications of thin layer chromatography, gas chromatography and liquid chromatography. Spectroscopic methods - forensic applications of ultraviolet-visible spectroscopy, infrared spectroscopy, atomic absorption spectroscopy, atomic emission spectroscopy. Mass spectrometry. X-ray diffraction. Colorimetric analysis of narcotics. Electrophoresis –forensic applications. Forensic photography- Basic principles and applications of photography in forensic science. 3D photography- Infrared and ultraviolet photography. ***Digital photography. Videography***.

5. NANOTECHNOLOGY IN FORENSIC CHEMISTRY 10 hours

Nanomaterials-Classification. Synthesis of nanomaterials-top-down and bottom-up synthesis - CVD. Application of nanotechnology in forensic evidence analysis- Collection and analysis of evidence of different types of crime scenes including explosive, drugs, DNA analysis, latent finger-marks.

References

1. W.J. Tilstone, M.L. Hastrup and C. Hald, Fisher's, *Techniques of Crime Scene Investigation*, CRC Press, Boca Raton (2013).
2. R. Saferstein, *Criminalistics: An Introduction to Forensic Science*, 13th Edition, Pearson Education, (2021).
3. M. Byrd, *Crime Scene Evidence: A Guide to the Recovery and Collection of Physical Evidence*, CRC Press, Boca Raton (2001).
4. S. B. Karch, *The Pathology of Drug Abuse*, CRC Press, Boca Raton (2002).
5. A. Poklis, Forensic toxicology in, *Introduction to Forensic Sciences*, 2nd Edition, W.G. Eckert (Ed.), CRC Press, Boca Raton (1997).
6. D.R. Redsicker, *The Practical Methodology of Forensic Photography*, 2nd Edition, CRC Press, Boca Raton (2001).
7. C. P. Poole, Jr. F. J. Owens, Introduction to nanotechnology, A John Willey & sons, INC., Publication (2003).
8. V. Chauhan, V. Singh, A. Tiwari, Applications of nanotechnology in forensic investigation, *Int. J. Life. Sci. Scienti. Res*., 2017, 3, 1047-1051.
9. L. Gabrielli, D. Rosa-Gastaldo, M.-V. Salvia, S. Springhetti, F. Rastrelli, F. Mancin, Detection and identification of designer drugs by nanoparticle-based NMR chemosensing, Chem. Sci., 2018, 9, 4777–4784.
10. S. J. Kwon, A. J. Bard, DNA Analysis by application of Pt nanoparticle electrochemical amplification with single label response, *J. Am. Chem. Soc.* 2012, 134, 26, 10777–10779.

11. W. Kemp, *Organic Spectroscopy*, 3rd Edition, Macmillan, Hampshire (1991).
12. Fundamentals of Molecular Spectroscopy by Colin N Banwell and Leaine McCash, Fourth Edition-2017, McGraw Hill Education Pvt. Ltd.

Semester	IV
Paper code	CHDE 0525
Paper title	Dept. elective: SUPRAMOLECULAR 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. INTRODUCTION TO SUPRAMOLECULAR CHEMISTRY (6 + 2) hours

Definition and development of supramolecular chemistry- lock and key analogy**,** cooperativity-pre-organisation-complementarity-thermodynamic, kinetic selectivity-nature of supramolecular interactions- solvation effects, supramolecular concepts and design. Host-guest chemistry. Synthesis: The template effect and high dilution.

Lariat ethers, podands, cyclodextrins cyclophanes, cryptophanes, carcerands, hemicarcerands.

Anion binding: Concepts in anion host design, different types of anion hosts. Simultaneous cation and anion binding. Cation-binding: crown ethers, cryptands, spherands, calixarenes (review-recall)

2. NATURE OF SUPRAMOLECULAR INTERACTION 3 hours

Ion-ion interactions, ion-dipole interaction, dipole-dipole interaction, hydrogen bonds, hydrophobic interactions.

3. CRYSTAL ENGINEERING 10 hours

Self-assembling capsules, molecular containers, metal directed capsules, hydrogen bonded capsules, concepts in crystal engineering, The Cambridge structural database, crystal engineering with hydrogen bonds, pi interactions - halogen bonding and other weak interactions, co-crystal, salts, polymorphs and their physico-chemical properties, coordination polymers. Solid state reactivity: metal-organic frameworks, guest properties of metal-organic frameworks.

4. SOLID STATE SUPRAMOLECULAR CHEMISTRY **8 hours**

Zeolites: structure, composition and catalysis. Clathrates: urea/thiourea clathrates, trimesic acid clathrates, clathrate hydrates (structure and function of the above species), uses. Inclusion compounds, intercalation compounds.

5. SELF-ASSEMBLY **12 hours**

Self-assembly in synthetic systems: pi-electron donor-acceptor systems, transition metal directed assemblies, hydrogen bond assemblies, anion directed assemblies, catenanes, rotaxanes, helicates, helical assemblies and molecular knots.

Guest binding by cavitands - calixarenes, resorcarenes, glycourils, cyclodexdrins; molecular clefts, tweezers, cyclophanes, cryptophanes, carcerends and hemicarcerends.

Molecular devices: Photo-switchable devices. Applications of supramolecular chemistry in sensors, switches and molecular machinery and molecular biology.

6. BIOLOGICAL MIMICS AND SUPRAMOLECULAR CATALYSIS **3 hours**

Characteristics of biological models. Supramolecular catalysis: cyclodexdrin as enzyme mimics.

7. SURFACTANTS AND INTERFACIAL ORDERING **3 hours**

Micelles and vesicles, surface self-assembled monolayers**.** Application to medicinal chemistry**.** Soft lithography, microlens arrays, transfer printing.

8. DENDRIMERS **5 hours**

Synthesis - divergent and convergent methods, host-guest chemistry of dendrimers. Supramolecular dendrimer assemblies. Applications of dendrimer for drug delivery.

9. NANOMATERIALS WITH SUPRAMOLECULAR STRUCTURE **8 hours**

Nanorod, nanowire self-Assembly: metal templating nanowires. Self-assembling nanorods. nanorod devices – nanotubes from nano porous templates. VLS synthesis of nanowires, nanowire quantum size effects. Manipulating nanowires, nanowire sensors.

Nanocluster self-assembly: synthesis of metal capped semiconductor nanoclusters, electrons and holes in nanocluster boxes, nanocrystal semiconductor alloys, nanocluster phase transition water soluble nanoclusters. Polymer nanocomposites.

REFERENCES:

1. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley, 2nd Edn., (2009).

2. Core Concepts in supramolecular Chemistry and Nanochemistry, J. W. Steed, T. R. Turner and K. J. Wallace, John Wiley & Sons, (2007).
3. Supramolecular Chemistry, L.-M. Lehn, VCH, 1995.
4. Crystal Design: Structure and Function, G. R. Desiraju (Ed.), John Wiley and Sons, (2003).
5. Supramolecular Chemistry: An Introduction Vögtle, F. John Wiley & Sons (1993).
6. Concepts of Modern Catalysis and Kinetics, I. Chorkendorff, J. W. Niemantsverdriet, Second Edition, Wiley-VCH Publishers, 2007.
7. Supramolecular chemistry (Oxford university press, 1999) P. D. Beer, P A Gale, D. K. Smith.

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 35% portions from the mid semester exam portion and 65% 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