ST JOSEPH'S UNIVERSITY

BENGALURU - 27

SCHOOL OF CHEMICAL SCIENCES

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ANALYTICAL CHEMISTRY

2026-2029

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 2026 ONWARDS

Department of Chemistry

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

Mission statement:

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

Benchmark Statements for the Course:

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

Teaching-Learning:

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

Co-curricular Activities:

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

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

SUMMARY OF CREDITS

SEMESTER: I	PAPER CODE AND TITLE	NO. OF TEACHING HOURS/week	NO. OF CREDITS	TOTAL MARKS
THEORY				
Paper I	CH7126: Inorganic Chemistry – I	4	04	100
Paper II	CH7226: Organic Chemistry – I	4	04	100
Paper III	CH7326: Physical Chemistry-I	3	03	100
Paper IV	CH7426: Spectroscopy -I	4	04	100
Paper V	CH7526: Principles of Chemical Analysis	4	04	100
PRACTICAL				
Paper I	CH7P126: Inorganic Chemistry Practical	4	02	50
Paper II	CH7P226: Chemical Analysis	4	02	50
Paper III	CH7P326: Organic Chemistry Practical	4	02	50
Paper IV	CH7P426: Applied Analysis	4	02	50
		TOTAL	**27**	**700**

SEMESTER II	PAPER CODE AND TITLE	NO. OF TEACHING HOURS	NO. OF CREDITS	TOTAL MARKS
THEORY				
Paper I	CH8126: Inorganic Chemistry II	4	04	100
Paper II	CH8226: Organic Chemistry II	4	04	100
Paper III	CH8326: Physical Chemistry II	4	04	100
Paper IV	CH8426: Spectroscopy II	4	04	100
Paper V	CH8526: Separation Techniques	3	03	100
PRACTICAL				
Paper I	CH8P126: Physical Chemistry Practical I	4	02	50
Paper II	CH8P226: Physical Chemistry Practical II	4	02	50
Paper III	CH8P326: Synthesis and characterization – I	4	02	50
Paper IV	CH8P426: Synthesis and characterization - II	4	02	50
		TOTAL	**27**	**700**

SEMESTER III	PAPER CODE AND TITLE	NO. OF TEACHING HOURS	**NO. OF CREDITS**	TOTAL MARKS
THEORY				
Paper I	CH9125: Biological Chemistry	4	04	100
Paper II	CH9225: Organometallic Chemistry	3	03	100
Paper III	CH9325: Electrochemistry and Electroanalytical Techniques	4	04	100
Paper IV	CH9425: Solid State Chemistry	4	04	100
Paper V	CH9525: Applied Analysis	4	04	100
PRACTICAL				
Paper I	CH9P125: Applied Analysis-I	4	02	50
Paper II	CH9P225: Applied Analysis-II	4	02	50
Paper III	CH9P325: Advanced Methods of Analysis –I	4	02	50
Paper IV	CH9P425: Advanced Methods of Analysis –II	4	02	50
		TOTAL	**27**	**700**

SEMESTER IV	PAPER CODE AND TITLE	NO. OF TEACHING HOURS	NO. OF CREDITS	TOTAL MARKS
THEORY				
Paper I	**Department Electives** CHDE 0225: Chemistry of Materials CHDE 0325: Green Chemistry and Diversity of its Applications CHDE 0425: Forensic Chemistry CHDE 0525: Supramolecular Chemistry	4	04	100
	CH0PR PROJECT WORK IGNITORS/ OUTREACH	35/week	10 04	200
		TOTAL	**18**	**300**

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

CREDITS FOR M.Sc. CHEMISTRY						
I -II SEMESTER						
	T/P	**Number Of Teaching Hours Per Week**	**CREDITS**	**Total Teaching Hours per Semester**	**TOTAL CREDITS IN ONE SEMESTER**	**TOTAL CREDITS IN ALL SEMESTERS**
Optional Subjects					27	27 x 2 = 54
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	2	50		
Practical –II	P	4	2	50		
Practical-III	P	4	2	50		
Practical –IV	P	4	2	50		
III SEMESTER						
Optional Subjects					27	27
A	T	4	4	60		
B	T	4	4	60		
C	T	3	3	45		
D	T	4	4	60		
E	T	4	4	60		
Practical-I	P	4	2	50		
Practical –II	P	4	2	50		
Practical-III	P	4	2	50		
Practical –IV	P	4	2	50		
IV SEMESTER						
Dept. elective	T	4	4	60	18	18
PROJECT	P	35	10	300		
IGNITORS/ OUTREACH			4			
TOTAL						**99**

FIRST SEMESTER

THEORY PAPERS

Semester	I
Paper code	CH 7126
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 **8+2 hours**

Molecular orbital theory: ***(Introduction to wave functions for molecular orbitals, LCAO approach)***, heteronuclear diatomic molecules/ions (NO, NO^-, CN^-, OH^-, and ICl). Polyatomic molecules – molecular orbitals of BeH_2 and NH_3, metal-metal bonding (MOT approach); metal-metal single and multiple bonded compounds (Cr, ***W, Re*** metal compounds), hypervalence in the context of molecular orbitals (SF_6), molecular shapes in terms of molecular orbitals - Walsh diagram (for XH_2 molecules: BeH_2, H_2O), calculation of bond enthalpy, Ketelaar triangle, Bent's rule, quadruple, quintuple and agostic bonds with examples.

2. THE STRUCTURES OF SIMPLE SOLIDS **18+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 phosphorus and sulphur: 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. 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. Silicon-Silicon (sil-ane, -ene, -yne) multiple bonded systems. Applications of main group elements in ***sustainable catalysis, organic synthesis, emerging materials,*** metallo-mimetic alternatives, carbon quantum dots, high-energy materials, radical and low-valent chemistry.

4. ACIDS AND BASES 5 + 1 hours

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-Acid-base pair: Use in small molecule (H_2) activation.

5. NONAQUEOUS SOLVENTS 4hours

Chemistry in non-aqueous media - Acid-base reactions in BrF_3 and N_2O_4. Molten salts -

Classification, properties and applications. Ionic liquids-preparation of 1-butyl-3-methylimidazolium hexafluorophosphate, properties and applications of ionic liquids. Reactions in supercritical fluids.

REFERENCES

1. Inorganic Chemistry, Weller, Rourke, Overton, 7th Edn., Oxford Univ. Press, 2018.
2. Inorganic Chemistry, Catherine E. Housecroft and Alan G. Sharpe, 5th Edn., Pearson Education Ltd., 2018.
3. Foundations of Inorganic Chemistry, Gary Wulfsberg, University Science Books 2018.
4. Fundamental Concepts of Inorganic Chemistry, Asim K Das, 3rd Edn., CBS, 2020.
5. Supercritical Fluids as Solvents and Reaction Media- G. Brunner, Elsevier, 2004.
6. Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edn., J.E. Huheey, E.A. Keiter and R.L. Keiter, Okhil. K.Medhi, Pearson Education Asia Pvt. Ltd. 2006.
7. Basic Inorganic Chemistry - F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and Sons, 3rd Edn., 1995.
8. Concise Inorganic Chemistry, J. D. Lee, 5th Edn., Blackwell Science, 2008.
9. Chemistry of Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann 1997.
10. Chemistry of non-metals, R. Stuedel, D. Scheschkewitch, Walter de Gruyter GmbH 2020.
11. Enantioselective Main Group Catalysis: Modern Catalysts for Organic Transformations, Lewis C. Wilkins, Rebecca L. Melen, Coord. Chem. Rev., 2016, 324, 123-139.
12. Organoboron-based multiple-resonance emitters: synthesis, structure–property correlations, and prospects, Masashi Mamada, Masahiro Hayakawa, Junki Ochi, Takuji Hatakeyama, Chem. Soc. Rev., 2024, 53, 1624.
13. Ruksana Akhtar, Kumar Gaurav, Shabana Khan, Applications of low-valent compounds with heavy group-14 elements, Chem. Soc. Rev., 2024,53, 6150-6243.
14. Advancing metallomimetic catalysis through structural constraints of cationic P^{III} species, Deependra Bawari, Donia Toami, Roman Dobrovetsky, Chem. Commun., 2025, 61, 5871.
15. Carbon quantum dots: properties, preparation, and applications, Jichuan Kong, Yihui Wei, Feng Zhou, Liting Shi, Shuangjie Zhao, Mengyun Wan, Xiangfeng Zhang, Molecules 2024, 29, 2002.

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

LO1	Knowledge	Recall concepts, laws, relationships, molecular structures in chemical bonding, crystal structures in solid state, and molecular orbital theory 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 molecular orbitals, close packing of spheres, and holes in a close-packed structure.
LO2	Understand	Explain hypervalence using hybridisation, magnetic properties using MOT, Structures of metals and alloys, bonding in boranes and phosphazenes; the properties of non-aqueous solvents, 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. 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. Apply molecular orbital theory to construct qualitative MO diagrams

		for dinuclear metal complexes containing single, double, triple, quadruple, and quintuple metal–metal bonds.
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 and metallocarboranes. Distinguish between single and multiple metal–metal bonds by analyzing orbital overlap, symmetry, and electron occupancy in dinuclear systems.
LO5	Evaluate	Compare the structure-property correlation in allotropes of S and P. Interpret the photoelectron spectrum to correlate the MO energies for a compound. Deduce the structure of carborane from the given higher borane. Assess the type of acid-base nature of the given compound
LO6	Create	Predict the formula of boranes from the given data. Propose the STYX number of a given borane.

Semester	I
Paper Code	CH 7226
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 in bold, italics, and underline corresponds to self-study

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

1. STRUCTURE, REACTIVITY & REACTION MECHANISMS 11+1 h

(Resonance, hyperconjugation), steric effects and steric inhibition of resonance on reactivity,

Quantitative treatment of field and resonance effects – Linear free energy relationship; 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 carbenes and nitrenes.

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

2. STEREOCHEMISTRY 17+2 h

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**,** systems with pseudoasymmetric centres. Stereochemistry of catenanes, rotaxanes, knots, and Mobius strips; cycloenantiomerism.

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 di-substituted ethanes. Conformation and configurational details of di-substituted cyclohexanes.

Fused rings and bridged rings, special features of their stereochemistry, conformational transmission, nomenclature of bridged systems, decalins: cis and trans decalins. norbornanes, bicyclo [2.2.2] octane, propellanes, adamantanes.

3. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 8+1 h

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. Neighboring group participation, non-classical carbocations. S_Ni mechanism. Allylic rearrangements.

Substitution at a trigonal carbon atom: Cleavage of esters and N-acylation reactions. Substitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

4. ELIMINATION REACTIONS 7+2 h

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. Case Study: Industrial dehydrogenation reaction.

Pyrolytic eliminations: Hofmann elimination, elimination in esters, xanthates and N–oxides - mechanisms and orientation.

5. AROMATIC SUBSTITUTION 9+2 h

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. Case study: Industrial alkylation reaction.

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

REFERENCES

1. Organic Chemistry, Clayden, Greeves, Warren and Wothers, 2nd Edn, Oxford university press, 2012.
2. March's advanced organic chemistry: Reactions, Mechanisms, and Structure, M. B. Smith, 8th Edn, John Wiley& Sons Inc., 2020.
3. Guidebook to Mechanism in Organic Chemistry (6th Edn), P. Sykes, Pearson education limited, 2003.
4. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley, 1994.
5. Stereochemistry of organic compounds, D. Nasipuri, 4th edition, New Age International publishers, 2021.
6. Advanced organic chemistry, Part A, F. A. Carey and J. Sundberg, 5th Edn., Springer, 2007.
7. Organic chemistry, Volumes I and II, I. L. Finar, 6th edition, Longman, 2002.

Learning outcomes: After learning this paper, students 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 7326
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 9 hours

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

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

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

2. QUANTUM MECHANICAL TREATMENT OF SIMPLE SYSTEMS 12hours

Quantum mechanical treatment of a free particle and a particle in a 1D/3D potential well; eigen values and normalized eigen functions, nodes, symmetry and anti-symmetry 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 confinement; 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 7 hours

Variation theorem and its proof; application to the ground state of helium atom.

Perturbation theory (time-independent); application of perturbation method to the ground state of helium atom (first order correction only).

Multielectron atoms – symmetric and antisymmetric wave functions; ground and excited states of helium; spin orbitals and Pauli principle; Slater determinants; Slater orbitals; effective nuclear charge based on Slater's rules.

4.THEORY OF ANGULAR MOMENTUM 4 hours

Commutation relationships among angular momentum operators; quantum mechanical definition of angular momentum;

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

5.CHEMICAL BONDING IN DIATOMIC AND POLYATOMIC MOLECULES

9+4 hours

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, sixth edition, New Age International (P) Ltd., 2025.
2. Quantum Chemistry, D. A. McQuarrie, Viva Books Pvt Ltd., 2016.
3. Quantum Chemistry, I. N. Levine, Prentice Hall, India, 2016.

4. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 4th Edition, Oxford University Press, 2005.
5. Introduction to Quantum Chemistry, A. K. Chandra, 4th Edition, Tata McGraw- Hil, 1994.
6. Physical Chemistry-Quantum Mechanics, Horia Metiu, Taylor & Francis, 2006.
7. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.

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

LO1	Knowledge	Recall the basic principles of quantum mechanics (QM), such as wave-particle duality and the Heisenberg uncertainty principle, quantization and matter waves. Define the fundamental QM operators such as position, momentum, and energy operators.
LO2	Understand	Explain the postulates, laws and relationships in QM, probability densities, eigen values, Schrödinger equation (SE), normalization and orthogonalization of wave functions, principle of chemical bonding, valence bond and molecular orbital theories. Describe the approximation methods used in QM, the assumptions of Huckel molecular orbital (HMO) theory. Understand how electrons interact within atoms and molecules. Summarize the electronic structure of atoms and molecules based on QM principles.
LO3	Apply	Setup and solve Schrödinger equation for simple systems, plot energy levels, problems involving quantum mechanical operators and their eigenstates. Calculate the energy of complex systems using approximation methods Predict the orbital functions and angular momenta of QM systems. Determine the microstates or terms of atomic orbitals. Apply the principles of QM to calculate energy levels, wave functions, and expectation values for simple systems. Use of QM concepts to predict the bond lengths and strengths. Derive HMO for simple conjugated systems.
LO4	Analyse	Differentiate between various QM models and their applications in

		chemistry, such as the particle in a box model and the harmonic oscillator model. Compare and contrast QM solutions for systems with the corresponding classical mechanical solutions, approximation methods and theories of bonding. Correlate the atomic terms to elucidate spectroscopic data.
LO5	Evaluate	Assess the validity of a QM model/method for a given system, the accuracy of QM calculations by comparing theoretical results such as energy, ionisation potential, dissociation energy with experimental data. Justify the need for rules such as $n+l$ rule, exclusion principle and Hund's rule. Evaluate the strengths and limitations of valence bond theory to predict the ionisation, chemical bonding and resonance structures of systems.
LO6	Create	Construct and solve Schrodinger equation for any given (hitherto unknown) system. Construct determinantal form of wave functions for any conjugated system Build the molecular orbitals of any π-system by HMO method.

Semester	I
Paper code	CH 7426
Paper title	SPECTROSCOPY – I
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

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

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

1. GROUP THEORY IN CHEMISTRY **17+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 Sn 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 nonrigid rotor. Rotational spectra of polyatomic molecules - linear, and symmetric top molecules. Calculation of bond length of diatomic and linear triatomic molecules. Stark effect.

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

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

4. RAMAN SPECTROSCOPY **7+1 hours**

Classical 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 orbitals and the spectra of ethylene.

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

Case study: Applications of Fluorescence spectroscopy in quinine

REFERENCES

1. Chemical Applications of Group Theory, An Indian Adaptation, 3rd Edn., F. Albert Cotton, Wiley Eastern, 2020.
2. Fundamentals of Molecular Spectroscopy, 6th Edn., C.N. Banwell, M. McCash, Affiliated east-west press, 2024.
3. Introduction to Molecular Spectroscopy, Gordon M. Barrow, Hassell Street Press, 2021.
4. Molecular Spectroscopy, Revised 1st Edn., J. D. Graybeal, McGraw Hill, 2014.
5. Modern Spectroscopy, 4th Edn., J. Michael Hollas, John Wiley, 2010.
6. Vibrational Spectroscopy, D.N. Sathyanarayana, First Edn., New Age International (P) Ltd. 2004.
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.
9. Symmetry and Spectroscopy of Molecules, Revised second Edn., New Age Publishers, 2020.
10. Harcher A., Ricard C., Connolly D., Gibbs I., Shaw J., Butler J., Perschbacher J., Replogle L., Eide M., Grissom M., O'Neal O., Nguyen Q., Nguyen V.H., Hunnicutt M., Mahmoud R., Dhakal S. Fluorescence Analysis of Quinine in Commercial Tonic Waters. *Methods Protoc.* 2025 Jan 6;8(1):5. https//doi:10.3390/mps8010005

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

LO1	Knowledge	Define point groups, groups and subgroups, order, symmetry elements (Identity, plane of symmetry, proper axis, improper axis, inversion center) and symmetry operations, harmonic and anharmonic oscillators and vibrational energy, rotational energy expression and its components, Frank-Condon principle, Born-Oppenheimer

		approximation, predissociation, dissociation energy in electronic states. Write examples of conjugate relationships, classes of operations and order of a group, the great orthogonality theorem. List the various symmetry elements for C2v, C3v 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 (C2v and C3v) 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 C2v and C3v 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	Analyse	Compare molecular structures (AB2 and AB3) based on Raman vibrational modes, the spectrum of rigid and non-rigid rotor. Compare and contrast the spectra of different diatomic molecules. Analyse 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.

Semester	I
Paper Code	CH7526
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 3 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 hour

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. Analytical applications - turbidimetric titrations.

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 4 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. Applications and case-study based thermogram analysis in polymer stability, pharmaceutical screening, and material characterization using DSC, DTA, and TGA.

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.

11. Giron, D. (2002). Applications of thermal analysis and coupled techniques in pharmaceutical industry. *Journal of Thermal Analysis and Calorimetry*, **68**, 335–357.

12. Gallagher, P. K. *Inorganic Systems, Thermal Analysis Applications to*. Encyclopedia of Analytical Chemistry, Wiley, 2006.

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

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

Semester	I
Paper code	CH7P126
Paper title	INORGANIC CHEMISTRY PRACTICAL
Number of teaching hours per week	4
Total number of teaching hours per Semester	44
Number of credits	2

1. 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).
   Instruction and demonstration of acid and basic radicals and model salt – (1 session)
2. Salt mixture analysis -1 (Acid radicals)
3. Salt mixture analysis -1 (Basic radicals)
4. Salt mixture analysis-2 (1 session)
5. Determination of alkalinity of waste/raw water samples.
6. Determination of total suspended solids in waste/raw water samples.
7. Synthesis and characterisation of perovskites: Synthesis (1 session)
8. Synthesis and characterisation of perovskites: Characterisation (1 session)
9. TECHNICAL IMMERSION: ADVANCED INORGANIC RESEARCH & INDUSTRIAL OPERATIONS: 2 sessions

   Field visit to Academic Centers of Excellence and Industrial Quality Control (QC) units.

   OR

   Industry-academia conferences/ seminar/ workshops. [Report submission]
10. Repetition/ Viva- 1 session.

REFERENCES

1. Vogel's Qualitative Inorganic Analysis, G. Svehla and B. Sivasankar, 7th Edition, Pearson

Education India, 2023.

2. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, , J. D. Barnes, M. J. K. Thomas, and B. Sivasankar, 6th Edition, Pearson Education, 2009.

3. Advanced Practical Inorganic Chemistry, Gurdeep Raj, 9th Edition, Goel Publishing House, 2020.

4. Standard Methods for the Examination of Water and Wastewater, William C. Lipps, Ellen B. Braun-Howland, and Terry E. Baxter (Eds.), 24th Edition, American Public Health Association (APHA), 2023.

5. Manual of Methods of Analysis of Foods – Water, Food Safety and Standards Authority of India (FSSAI), 1st Edition, FSSAI, 2024.

6. Easy Synthesis of High-Purity BiFeO3 Nanoparticles: New Insights Derived from the Structural, Optical, and Magnetic Characterisation, JoséLuis Ortiz-Quiñ onez *et.al*., *Inorg. Chem.* 2013, 52, 10306−10317, DOI: dx.doi.org/10.1021/ic400627c.

11. Synthesis and Characterization of a Perovskite Barium Zirconate (BaZrO3): An Experiment for an Advanced Inorganic Chemistry Laboratory, Todsapon Thananatthanachon, *J. Chem. Educ.* 2016, 93, 1120−1123, DOI: 10.1021/acs.jchemed.5b00924.

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. Recall the definitions of phenolphthalein and methyl orange alkalinity. Identify the general ABX_3 crystal structure and the common precursors used. Identify the core functions of a Quality Control (QC) laboratory and Research R&D.
LO2	Understand	Explain the concept of solubility product and common ion effect. Explain the chemical reactions involved in acid-base neutralization of water.

		Distinguish between various types of hardness and metal ion interference. Explain the relationship between the Goldschmidt Tolerance Factor and the stability of the perovskite lattice. Explain the organizational hierarchy and safety protocols (GLP/GMP) in an industrial setting.
LO3	Apply	Perform analysis of cations and anions in salt mixture samples. Calculate the total alkalinity in terms of mg/L of $CaCO_3$ equivalents. Calculate the exact stoichiometric masses required to produce a specific molarity of perovskite precursor solution. Relate classroom chemical theories to the large-scale industrial operations observed.
LO4	Analyze	analysis of salt mixture samples containing more number of cations and anions. Correlate TSS levels with potential sources of industrial or domestic pollution. Compare experimental results with FSSAI safety standards. Interpret XRD patterns to identify crystal phases and calculate the lattice constant (a). Examine the workflow of an Industrial QC unit and identify how it differs from academic research. Compare the sensitivity and throughput of industrial instruments (like ICP-MS) vs. lab titration.

LO5	Perform	Practice strict safety protocols, understand the handling of hazardous chemicals. Execute the gravimetric filtration and drying process for TSS determination. Execute the spin-coating or antisolvent precipitation method to synthesize a thin film or powder sample. Document observations systematically during the site visit or conference sessions.
LO6	Evaluate	Compare systematic analysis with spot tests. Assess the precision of titrimetric results using triplicate analysis. Compare the experimental optical bandgap (from a Tauc Plot) against theoretical literature values. Assess the importance of regulatory compliance in maintaining product quality and public safety.
LO7	Create	Develop a protocol to do qualitative and quantitative analysis of given samples containing cations and anions. Design a standardized SOP for testing raw water quality in a local area. Design a modified recipe to shift the bandgap. Formulate a professional technical report or presentation summarizing the immersion experience.

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Semester	I
Paper code	CH7P226
Paper title	CHEMICAL ANALYSIS
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	2

CHEMICAL ANALYSIS : **11 Sessions**

1. Statistical analysis (Including least square analysis). (2 sessions)
2. Estimation of sulphate concentration using turbidimeter.
3. Determination of turbidity of the given sample using nephelometer.
4. Gravimetric and volumetric analysis of either Fe and Al or Cu and Ni (2 sessions)
5. Estimation of caffeine in a given sample using UV spectrophotometer.
6. Estimation of a mixture of Fe and Sn by potentiometry.
7. Determination of quantum yield and calculation of Stokes shift using UV-Visible and fuorescence spectroscopy.
8. Estimation of sodium/potassium/lithium by flame photometer.
9. Estimation of alkali metals in a given mixture by flame photometer.
10. Estimation of mixture of halides by potentiometry.
11. Auto-titration
12. Estimation of Halides by Mohr's or Volhard's method .
13. Analysis of trace elements in petrochemicals by spectrophotometry and colorimetry

REFERENCES

1. Soffiantini, V. A. (2021). *Analytical Chemistry: Principles and Practice*. De Gruyter. ISBN: 9783110721195.
2. Mendham, J., Denney, R. C., Barnes, J. D., & Thomas, M. J. K. (Eds.). (2009). *Vogel's textbook of quantitative chemical analysis* (6th ed.). Pearson Education. ISBN 9780582226289..
3. Khosla, B. D.,Garg, V. C. and Gulati, A. Senior Practical Physical Chemistry, R.

Chand and Co. (2011).

4. Garland, C. W., Nibler, J. W. and Shoemaker, D. P. Experiments in Physical Chemistry, 8th Ed, McGraw-Hill: New York (2003).
5. 4. Halpern, A. M. and McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman and Co., (2003).
6. Seedher, N. (2023). *A comprehensive guide to physical chemistry experiments and viva questions* (2nd ed.). Notion Press. ISBN: 979-8891861916
7. Singh, J., Yadav, L. D. S., Singh, R. K. P., Siddiqui, I. R., Singh, J., & Srivastava, J. (2022). *Advanced practical chemistry* (10th ed.). Pragati Prakashan.Malati, M. A. (1999; reprinted 2010).
8. Nadkarni, R. A. K. (2005). Elemental analysis of fuels and lubricants: Recent advances and future prospects. ASTM International. https://doi.org/10.1520/stp1468-eb
9. 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.
10. 2. Principles of Instrumental Methods of Analysis,7thEdn., D. A. Skoog, F. J. Holler, S. R. Crouch, Cengage India Pvt. Ltd., 2020

Learning Objectives: At the end of the course the student should be 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, Recall fundamental principles of analytical, physical, and inorganic chemistry techniques. Memorize standard procedures for gravimetric, volumetric, turbidimetric, spectrophotometric, potentiometric, and flame photometric experiments. Identify laboratory equipment and reagents used in each experiment; sources of error and evaluate their impact on experimental outcomes. Record the details of an experiment performed.

LO2	Understand	Explain statistical tools (mean, standard deviation, least squares) and their relevance to experimental data, auto-titration mechanisms. Describe the principles of light scattering (turbidimetry/nephelometry), Beer–Lambert's law, fluorescence, potentiometry, and flame photometry.precipitation titrations (Mohr's and Volhard's) Interpret experimental observations and relate them to theoretical concepts. .
LO3	Apply	Perform quantitative analysis using gravimetric, volumetric, spectrophotometric, potentiometric, and flame photometric techniques. Construct calibration curves and determine concentrations of unknown samples. Apply statistical analysis to experimental data for validation of results. Use auto-titrators and modern lab instruments to improve accuracy and reproducibility.
LO4	Analyze	Compare results obtained by classical and instrumental methods. Identify sources of error and evaluate their impact on experimental outcomes. Analyze titration curves, absorption/emission spectra, and turbidity measurements to locate equivalence points or critical values. Interpret overlapping or interfering signals in mixtures of metals or halides.
LO5	Evaluate	Compare results obtained by classical and instrumental methods. Analyze titration curves, absorption/emission spectra, and turbidity measurements to locate equivalence points or critical values.

		Interpret overlapping or interfering signals in mixtures of metals or halides.
LO6	Create	Design improved experimental procedures to minimize error or enhance efficiency. Integrate multiple analytical methods to solve complex mixture analysis problems. Formulate data interpretation reports that combine statistical, graphical, and theoretical analysis. Propose new approaches to practical problems in inorganic and physical chemistry laboratories.

Semester	I
Paper Code	CH7P326
Paper Title	ORGANIC CHEMISTRY PRACTICAL
Number of Teaching Hours per Week	4
Total Number of Teaching Hours per Semester	44
Number of Credits	2

List of experiments: (11 sessions)

1. Separation, systematic analysis and identification of organic compounds in a binary mixture. (6 Sessions)
2. Determination of equivalent weight of carboxylic acids.
3. Estimation of phenols by bromination method.
4. Determination of Iodine value of oil/fat
5. Estimation of reducing and non-reducing sugar in a mixture
6. Estimation of acetone by Iodometry.
7. Repetition lab/viva

References:

1. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari, Allied Publishers, 2nd edition, 1996.
2. Practical Organic Chemistry, Mann and Saunders, 4th edition (reprinted), ELBS / Longman, London, 1980.
3. Textbook of Practical Organic Chemistry, A.I. Vogel, 5th edition, 1996.
4. Textbook of Quantitative Organic Analysis, A.I. Vogel, 5th edition, 1996.
5. A Handbook of Organic Analysis, Clarke and Hayes, 5th edition, 1964.
6. A Handbook of Organic Analysis: Qualitative and Quantitative, Clarke, Haynes, Brick and Shone, 1975.

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. 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	Explain the principles and procedures involved in qualitative analysis, including separation techniques and chemical tests for identifying organic compounds. Describe the reactions involved during volumetric titration. Detail the concept of iodine value and its significance in lipid analysis. Explain the importance of calibration and standardization procedures in titration experiments.
LO3	Apply	Apply separation techniques, systematic analysis procedures and qualitative tests to effectively separate and identify organic compounds within binary mixtures. 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	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 Identify the amount of organic compound present in a sample. Interpret iodine value data to evaluate the quality of oils and fats.
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. Assess the feasibility of these methods in the estimation of structurally related organic compounds.
LO6	Create	Create innovative strategies, protocols, and frameworks for optimizing qualitative analysis procedures, including separation techniques and systematic qualitative analysis of organic molecules. Design the suitable method to estimate the amount of a given organic compound.

Semester	I
Paper Code	CH7P426
Paper Title	APPLIED ANALYSIS
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	2

11 sessions

1. Non-aqueous titration.
2. Analysis of alloy: Estimation of Iron in steel. (Session 1)
3. Estimation of Chromium in Steel. (Session 2)
4. Ion Exchange Chromatography: Preparation of Column. (Session 1)
5. Estimation of zinc and cadmium in the eluant. (Session 2)
6. Analysis of soil (Cation exchange capacity/ Organic matter)

Session 7 to 10: RBPT

11. Repetition lab/Viva.

References:

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

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

LO1	Knowledge	Define nonaqueous titration Identify nonaqueous solvents used in titration Recall the principle of non-aqueous titration Give the chemical reactions involved in various titrations
LO2	Understand	Extrapolate redox titration to estimate iron and chromium in steel Explain the importance of calibration and standardization procedures in titrations, the theoretical principle of Job's method Describe the role of each reagent in the various volumetric estimations
LO3	Apply	Employ experimental techniques specific to ion exchange chromatography, including column packing, sample loading, elution optimization, and detection methods Choose synthetic techniques specific to the preparation of ionic liquids, including the selection of appropriate cations and anions, reaction conditions, and purification methods Demonstrate skills in sample preparation techniques tailored to solvent extraction Apply Job's method to determine the stoichiometry of metal-ligand Complexes
LO4	Analyze	Analyze experimental data obtained from volumetric estimations and use it to determine the concentration of unknowns in a sample
LO5	Evaluate	Evaluate various techniques for determining the cation exchange capacity of soil samples Recommend suitable techniques for the characterization of synthesized Compounds
LO6	Create	Design suitable experiments for the preparation/ estimation of compounds by RBPT

SECOND SEMESTER
THEORY PAPERS

Semester	II
Paper Code	CH8126
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 corresponds 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+}).

4. MAGNETIC PROPERTIES OF METAL COMPLEXES 9+1 hours

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

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

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

Stereochemical non-rigidity, Stereoisomerism – chirality, optical activity, Circular Dichroism, Optical Rotatory Dispersion, Cotton effect and absolute configurations.
Concepts of Supramolecular Chemistry: Definition, nature of supramolecular interactions, host-guest interaction, molecular recognition, types of recognition, self-assembly.

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

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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	CH8226
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 corresponds 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, mechanisms of imine, oximes and hydrazones of carbonyl compounds, modified Wittig reaction, metal hydride reduction of carbonyl compounds and nitriles. Multicomponent reaction: Strecker Synthesis, Biginelli reaction, Knoevenagel–Michael addition/cyclisation. ***Case study: Multicomponent Biginelli reaction-assisted drug discovery***.

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION **4+1 hours**

SE1, SE2 and SEi mechanisms, hydrogen exchange, and migration of double bonds. Aliphatic diazonium coupling, nitrosation at carbon and nitrogen, diazo transfer reaction, 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.

Case study: Application of rearrangement reaction to Natural Product Synthesis and Modern Drug Discovery and Medicinal Chemistry.

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 rearrangements. 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.

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

LO1	Knowledge	Recall the nucleophilic, electrophilic addition reactions, multicomponent reaction; 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 the reaction mechanism
LO4	Analyze	Point out whether an acid or a base can be used to catalyse a reaction. Compare and contrast 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, multicomponent and rearrangement reactions

Semester	II
Paper Code	CH 8326
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 givenenergy 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, fugacity coefficient (ϕ), determination of fugacity by graphical, low pressure, and compressibility factor methods. 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 (ΔG_{mix}, ΔS_{mix}, ΔH_{mix} and ΔV_{mix}). Excess thermodynamic functions (G^E, S^E, V^E, H^E, and μ^E). Determination of 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 (dehydrogenation of ethane), 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

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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 overall formation of the product in the case of chain reactions iv) theory to predict the reaction rate on increasing the charge v) a steady-state hypothesis to predict the order of the reaction at low and high pressures if the mechanism of unimolecular reactions is given vi) Rice and Herzfeld mechanism for the kinetics of decomposition of acetaldehyde and ethane, vii) the

		conditions for the explosion and the explosion limits for the reaction between hydrogen and oxygen viii) quantitative and qualitative treatments of unimolecular reactions by Lindemann, Hinshelwood, RRK, and RRKM theories ix) Gibbs-Duhem-Margules equation to prove that in a binary solution if the solvent obeys Raoult's law then the gas obeys Henry's law x) Konovalov's laws to explain the principles of fractional distillation xi) chemical potential to validate phase rule xii) the partition function to compute thermodynamic properties of systems, such as internal energy, entropy, and free energy xiii) the concepts of partition function for different types of systems, including monoatomic and diatomic, xiv) the concept of partition function to explain Einstein's theory of heat capacity. **Construct** phenomenological equations for a process involving more than two fluxes and forces. **Prove** that the energy received by subsystem I from subsystem II is equal and opposite sign to that received by system II from I through the thermallyconducting surface. **Derive** an expression for entropy production i) in terms of fluxes and forces ii) in heat flow iii) matter flow and iv) in chemical reactions **Explain** kinetics of polymerization and by using radical mechanism and applying steady state. **Predict** i) the products based on the structure of the activated complex, extent of solvation, and effect on activity coefficient ii) the partition functions for a system containing a monoatomic gas iii) and interpret experimental results by applying the knowledge of primary and secondary salt effects. **Prove** that a loose vibrational motion ultimately gets converted to a translational motion.

		Evaluate the diffusion-controlled rate constant for the reaction between two molecules **Calculate:** the i) fraction of molecules having sufficient energy to react and form the product if activation energy for a reaction is given, along with the number of collisions ii) ionic strength of a solution iii) $\Delta^{\#}G^0$, $\Delta^{\#}H^0$, $\Delta^{\#}S^0$, and the pre-exponential factor for the reaction from the given data of rate constant, Ea, and T iv) the partial molal volume v) Calculate ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, and ΔH_{mix} for ideal and non-ideal solutions, vi) excess thermodynamic properties (G^E, S^E, H^E, V^E, and μ^E) vii) the nuclear partition function of the ortho hydrogen and para-hydrogen molecules viii) the translational partition function, rotational partition function andvibrational partition function. **Choose** the solvents in the increasing order of reaction rate between a pairof ions and explain the order of the arrangement. Formulate an expression for the consumption of a monomer. **Derive:** i) an expression for the rate constant using conventional transition state theory by treating the motion over the energy barrier as a loose vibrational ii) an expression for the rate constant using conventional transition state theory by treating the motion over the energy barrier as translational iii) thermodynamic formulation of conventional transition state theory and obtain an expression for the rate constant of an unimolecular reaction iv) an expression for rate constant and discuss the effect of internal pressure on reaction rates v) Henry's, Raoult's and Nernst distribution laws from chemical potential vi) an expression for apparent molar volume vii) ΔG_{mix}, ΔS_{mix}, ΔV_{mix}, and ΔH_{mix} for ideal and non-ideal solutions viii) Gibbs-Duhem equation ix) Gibbs-Duhem-Margules equation x) Konovalov's I and II law from Gibbs-Duhem-Margules equation xi) Sackur-Tetrode equation to determine

		translational entropy of a monoatomic gas xii) translational partition function, rotational partition function and vibrational for a monoatomic gas xiii) the expression for the distribution of particles using Maxwell-Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics xiv) relationship of the partition function with internal energy, entropy, Gibbs free energy, work function and enthalpy xv) an expression for equilibrium constant (K_p) in terms of partition functions, xvi) law of equipartition energy using partition function. **Determine:** i) activity and activity coefficient using emf and solubility measurements, ii) partial molal volume using reciprocal density method iii) partial molal volume using intercept method when mole fractionis given. Explain the effect of variation of temperature and pressure on chemical potential.
LO4	Analyze	**Analyze:** i) the factors influencing entropy production in different processes,such as heat flow, matter flow, and chemical reactions ii) the kinetics of chain reactions, such as the H_2 and O_2 reactions, and interpret explosion limits, iii) mechanisms such as the Rice-Herzfeld mechanism in thedecomposition of a molecule and predict the order of the reaction iv) the given mechanism and propose the order of the reaction in the case of decomposition of an organic molecule, apply steady state, and evaluate activation energy v) the stated conditions to predict the explosion and the explosion limits for the reaction between any two reactants vi) and predict the rates of reactions from the given data on ionicstrength. **Compare and contrast** i) different theories of unimolecular reactions to understand their strengths and limitations ii) RRK

		and RRKM theories. **Predict:** i) the reaction rates based on dielectric constants' data of solvents ii) the effect of solvation on the reaction rate for any reaction based on the solvent polarity. **Choose** the solvents in the increasing order of reaction rate between a pairof ions and explain the order of the arrangement. **Infer** the kinetics of polymerization by applying steady state and using a free radical mechanism. Justify the reaction outcomes by applying the concepts of kinetic and thermodynamic control. **Identify** the decrease in volume of solution after mixing two solvents. Correlate the decrease in the volume for a mixture of liquids to partial molal property. **Examine** the scale-up ratio required to obtain the desired volume aftermixing two solvents using the principles of partial molal volume. **Relate** macroscopic properties of systems to its microscopic states. Compare and contrast the predictions of statistical mechanics with those of classical thermodynamics.
LO5	Create	**Develop:** strategies to control reaction kinetics for desired outcomes in chemical processes, considering factors such as temperature, concentration,and solvent properties. **Arrive** at the molecular spectra from statistical thermodynamics. Apply the concepts of partition function for polyatomic molecules.
LO6	Evaluate	**Evaluate:** i) the significance of entropy production as a measure of irreversibility in natural and engineered systems ii) the features and characteristics of fast reactions and their significance in chemical processes, iii) partition functions from spectral data. **Critically evaluate** the methods used to study fast reactions,

		including flow,relaxation, flash photolysis, and NMR methods, in terms of their strengthsand limitations. Analyze the given data of different reactions, plot it on ln (k/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	CH8426
Paper title	SPECTROSCOPY – II
Total number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

Note: 1. Text in italics, bold and underlined corresponds to self-study.

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

1.INFRARED SPECTROSCOPY 5+2 hours

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.

2. 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 dienes and enones.

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 **8+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.*** Soft ionization and hard ionization techniques-ESI, APCI, APPI-Coulombic explosion, Rayleigh limit. Structure determination of molecules.

7.ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY **4 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).

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, 2025.

2. Vibrational Spectroscopy: Theory and Applications, 4th Edition D.N. Sathyanarayana, New-Age International publishers, New Delhi, 2024.

3. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore, 2001.

4. Physical Methods in Inorganic Chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi, 2025.

5. Applications of Absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, 2007.

6. Organic Spectroscopy, W. Kemp, ELBS London, 2022.

7. Spectrometric Identification of Organic Compounds, 8th Edition, R.M. Silverstein and W.P. Webster, Wiley & Sons, 2014.
8. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5th Edition, Saunders College Publishing, London, 2020.
9. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing, New York, 1992.
10. Mass Spectrometry - analytical Chemistry by Open Learning, 2nd Edition, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, 1998.

Course 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 λ_{max}. Elaborate on isotropic and anisotropic systems, zero-field splitting,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 (1H and 13C) 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 1H 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 1H 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 8526
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**

Liquid-liquid extraction/solvent extraction: partition coefficient, distribution ratio and percent extraction, choice of solvents. Equation for batch extraction and multiple extraction. Extraction efficiency - pH effects. Extraction with metal chelator and crown ethers. Separations based on complexation reactions (Masking). Multistage extraction. Craig's counter-current distribution.

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 splitless 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 2hours

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, Lloyd 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 KD, 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	CH8P126
Paper Title	PHYSICAL CHEMISTRY PRACTICAL - I
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	2

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.

(2 sessions)

2. Kinetics of reaction between $K_2S_2O_8$ and KI (salt effect) by volumetry.
3. Determination of rate constant for the oxidation of alcohol by colorimetry.
4. Determination of partial molal volume of ethanol by reciprocal density method.
5. Determination of partial molal volume by apparent molar volume method, NaCl-H_2O system
6. Determination of pK_a of indicators by colorimetry
7. Evaluation of rate constant of first order reaction by potentiometry.
8. Colorimetric estimation of aspirin.
9. Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$ using spectrophotometry.
10. Determination of Cu by colorimetry.
11. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.
12. Determination of solubility product of calcium hydroxide by saturation titration method.
13. Determination of the Fe by colorimetry.

12. Repetition/Viva

REFERENCES

1. Experiments in Physical Chemistry, Carl Garland, Joseph Nibler, and David Shoemaker and Garland, McGraw Hill International Edition, 2008.

2. Thermodynamics, Rajaram and J.Kuriacose, Shobanlal Publishers, 1999.

3. Findlay's Practical Physical Chemistry, revised by Levitt, Longman's, London, 1973.

4. 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	CH8P226
Paper Title	PHYSICAL CHEMISTRY PRACTICAL - II
Number of teaching hours per week	4
Total number of teaching hours per Semester	44
Number of credits	2

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
2. Estimation of urea by enzyme hydrolysis using conductance method.
3. Determination of dissociation constant of a weak acid by conductometry.
4. Determination of equivalent conductance and verification of Onsagar parameters for a strong electrolyte by conductometry. (1 session)
5. Determination of thermodynamic parameters of micellization of a surfactant from conductivity measurements.
6. Potentiometric estimation of extent of intercalation.
7. Titration of a weak dibasic acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid.
8. Titration of a mixture of strong and weak acids potentiometrically and the determination of the composition of the mixture.
9. Determination of activity coefficient of H^+ by potentiometry.
10. Determination of rate constant of saponification of ethyl acetate by conductometry
11. Degree of hydrolysis of aniline hydrochloride by potentiometry.
12. Determination of degree of hydrolysis and hydrolysis constant of ammonium chloride and sodium acetate conductometrically.
13. Redox titration of KI vs $KMnO_4$ using potentiometry
14. Repetition/Viva

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	CH8P326
Paper Title	SYNTHESIS AND CHARACTERIZATION OF COMPOUNDS- I
Number of Teaching Hours per Week	4
Total Number of Teaching Hours per Semester	44
Number of Credits	2

List of experiments: (11 sessions)

1. Preparation and quantitative analysis of hexamminecobalt(III) chloride. (2 sessions)
2. Preparation of potassium trioxalatoferrate(III) trihydrate and its characterization by quantitative analysis and IR studies. (2 sessions)
3. Preparation of a variety of complexes and their characterization by UV-Visible and IR techniques. (1 session)
4. Determination of stoichiometry of metal-ligand complex using Job's method. (1 session)
5. Preparation of a nano material/metal-organic framework and its characterization by UV spectroscopy (band gap). (2 sessions)
6. Synthesis of spinel and its characterization by XRD studies. (2 sessions)
7. Repetition/viva. (1 session)

References:

1. Quantitative Chemical Analysis; D. C. Harris, C. A. Lucy, 11th Ed., Macmillan Learning's, 2025.

2. Advanced Practical Chemistry; J. Singh, L. D. S. Yadav, R. K. P. Singh, I, R. Siddiqui, J. Singh, J. Srivastava, 2nd Ed., Pragati Prakashan, 2010.

3. Vogel's Textbook of quantitative chemical analysis; J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, 6th Ed., Pearson Education Limited, 2009.

4. Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A, B: 6th Ed., K. Nakamoto, John Wiley & Sons, 2009.

5. Integrated Approach to Coordination Chemistry, R. A. Marusak, K. Doan, S. D. Cummings, John Wiley & Sons, 2007.

6. Electronic Absorption Spectroscopy and Related Techniques, D. N. Sathyanarayana, Universities Press, 2001.

7. Experimental Inorganic/Physical Chemistry, M. A. Malati, Woodhead Publishing Limited, 1999.

8. Practical Inorganic Chemistry, G. Pass, H. Sutcliffe, Chapman and Hill, 1974.

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

LO1	Knowledge	Outline the method of preparation of square planar and octahedral complexes Write the protocol for the preparation of different coordination complexes/inorganic materials Record the details of the preparation of coordination complexes/inorganic materials and their spectral/volumetric analyses
LO2	Understand	Explain various factors that determine the formation of complexes/inorganic materials
LO3	Apply	Modify the reaction conditions for the preparation of various complexes/inorganic materials for comparative study Estimate of the constituents of complexes/inorganic materials based on the principles of volumetric analyses Compare the theoretical and experimental weight percentages of constituents of a complex
LO4	Analyze	Interpret the spectroscopic/XRD/TGA data of prepared complexes/inorganic materials, nature of bonding and types of transitions giving spectral bands Compare the UV/IR spectral data of cis and trans isomers
LO5	Evaluate	Predict the structure/properties of complexes/inorganic materials by IR/UV, TGA, DTA, XRD
LO6	Create	Develop new protocols/methods for the preparation of metal complexes of low (2-5) and high coordination numbers (7-10), geometrical isomers: tetrahedral, square planar, *cis- trans*, facial, meridional isomers of octahedral complexes

Semester	II
Paper code	CH8P426
Paper title	SYNTHESIS AND CHARACTERIZATION OF COMPOUNDS-II
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	2

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 anhydride (2 sessions)
4. Preparation of 2-iodoxy benzoic acid (IBX) from anthranilic acid and its application for the oxidation of alcohol (2 sessions)
5. Preparation of dibenzalacetone and reduction of carbonyl group (2 sessions)
6. Application of *N*-bromosuccinimide (NBS) in allylic bromination (1 session)

All the above synthesized compounds will be confirmed by TLC and spectral characterization.

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

QUESTION PAPER PATTERN-ESE

St. Joseph's University, Bengaluru-27
M.Sc. End-Semester Examination
(2026-29)
ANALYTICAL / ORGANIC CHEMISTRY

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

Instructions

1. The question paper has three Parts. Answer all the Parts.
2. Write chemical equations 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
(2026-29)
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**

EVALUATION PATTERN- THEORY

Continuous Internal Assessment	Activity 1+Activity 2	15 +15 = 30
	Mid sem Theory Exam	25 marks (converted to 20)
Total continuous Internal Assessment		50
End semester Theory examination		50
Total Marks		**100**