ST JOSEPH'S UNIVERSITY
Bengaluru-27

Syllabus for

4^{th} Year Honors Syllabus: B.Sc. Chemistry Honors

7^{th} Semester: NEP 2025

Department of Chemistry

School of Chemical Sciences

St Joseph's University

Bengaluru-560 027

Structure of the Chemistry course for I-VI semesters of BSc Degree

The B.Sc. honors degree course is a four-year program divided into eight semesters. Each semester will consist of 14 weeks of instruction for theory and 11 weeks of instruction for practicals. In Chemistry there will be 13 discipline core papers,6 discipline selective papers, 12 practical papers and a research proposal/project course from I to VIII semesters. For theory papers, internal assessment (CIA) is given 40% weightage and the end-semester examination (ESE) is given 60%. The practical internal assessment (PIA) is given 60% weightage and the end-semester practical examination is given 40%. The CIA is based on written tests, seminars, assignments, quizzes, etc. The end-semester theory examination is for 2-hour duration (60 marks) and the practical examination is for 3-hour duration (20 marks).

Semester	Code number	Title of the paper	No. of hours of instruction	No. of hours of teaching per week	Continuous internal assessment (CIA)	End semester marks	Total marks
I	CH124	Chemistry I	45	**3**	**40**	**60**	**100**
	CH1P24	Practical I	33	**3**	**30**	**20**	**50**
II	CH224	Chemistry II	45	**3**	**40**	**60**	**100**
	CH2P24	Practical II	33	**3**	**30**	**20**	**50**
III	CH325	Chemistry III	45	**3**	**40**	**60**	**100**
	CH3P25	Practical III	33	**3**	**30**	**20**	**50**
IV	CH425	Chemistry IV	45	**3**	**40**	**60**	**100**
	CH4P25	Practical IV	33	**3**	**30**	**20**	**50**
V	CH5126	Chemistry V-1	45	**3**	**40**	**60**	**100**
	CH5P1	Practical V-1	33	**3**	**30**	**20**	**50**
	CH5226	Chemistry V-2	45	**3**	**40**	**60**	**100**
	CH5P2	Practical V-2	33	**3**	**30**	**20**	**50**
	CH5326	Chemistry V-3	45	**3**	**40**	**60**	**100**
	CH5P3	Practical V-3	33	**3**	**30**	**20**	**50**

VI	CH6126	Chemistry VI-1	45	**3**	**40**	**40**	**100**
	CH6P1	Practical VI-1	33	**3**	**30**	**30**	**50**
	CH6226	Chemistry VI-2	45	**3**	**40**	**40**	**100**
	CH6P2	Practical VI-2	33	**3**	**30**	**30**	**50**
	CH6326	Chemistry VI-3	45	**3**	**40**	**40**	**100**
	CH6P3	Practical VI-3	33	**3**	**30**	**30**	**50**
VII	CHXXX	Chemical Analysis and Spectroscopy	45	**3**	**40**	**60**	**100**
	CHXXX	Practical-VII-1	33	**3**	**30**	**20**	**50**
	CHXXX	Advanced Organic Chemistry	45	**3**	**40**	**60**	**100**
	CHXXX	Practical-VII-2	33	**3**	**30**	**20**	**50**
	CHXXX	Coordination And Bioinorganic Chemistry	45	**3**	**40**	**60**	**100**
	CHXXX	Forensic Chemistry	45	**3**	**40**	**60**	**100**
	CHXXX	Industrial Chemicals, Analysis, Energy and Environment	45	**3**	**40**	**60**	**100**
	CHXXX	Supramolecular Chemistry	45	**3**	**40**	**60**	**100**
	CHXXX	Research Methodology	45	**3**	**40**	**60**	**100**

Summary of credits for I-VIII semesters

Semester	Code number	Title of the paper	No. of hours of teaching per week	Credit
I	CH124 CH1P24	Chemistry I Practical I	3 3	3 2
II	CH224 CH2P24	Chemistry II Practical II	3 3	3 2
III	CH325 CH3P25	Chemistry III Practical III	3 3	3 2
IV	CH425 CH4P25 CHMEXXX Multidisciplinary Elective:	Chemistry IV Practical IV Cosmetics and Personal Care Products	3 3	3 2
V	CH5126 CH5P1 CH5226 CH5P2 CH5326 CH5P3	Chemistry V-1 Practical V-1 Chemistry V-2 Practical V-2 Chemistry V-3 Practical V-3	3 3 3 3 3 3	3 2 3 2 3 2
VI	CH6126 CH6P1	Chemistry VI-1 Practical VI-1	3 3	3 2

	CH6226 CH6P2 CH6326 CH6P3	Chemistry VI-2 Practical VI-2 Chemistry VI-3 Practical VI-3	3 3 3 3	3 2 3 2
VII	CHXXX CHXXX CHXXX CHXXX CHXXX CHXXX CHXXX CHXXX CHXXX	Chemical Analysis and Spectroscopy Practical-VII-1 Advanced Organic Chemistry Practical-VII-2 Coordination And Bioinorganic Chemistry Forensic Chemistry Industrial Chemicals, Analysis, Energy and Environment Supramolecular Chemistry Research Methodology	3 3 3 3 3 3 3 3 3	3 2 3 2 3 3 3 3 3

Name of the Degree Program	B.Sc. (Honours)
Discipline Core	Chemistry
Total Credits for the Program	128+45(IV YEAR)=173

Assessment: Weightage for assessments (in percentage)

Type of Course	Formative Assessment / IA	Summative Assessment
Theory	40	60
Practical	60	40

Semester	**VII**
Paper code	**CHXXXX**
Paper title	**CHEMICAL ANALYSIS AND APPLIED SPECTROSCOPY**
Number of teaching hrs per week	**3**
Total number of teaching hrs per semester	**45**
Number of credits	**3**

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

STATISTICAL DATA TREATMENT AND EVALUATION 9+1 hours

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, and 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. Validation and reporting of analytical results: Sample, method and data validations, importance of following GLP to publish results. (***<u>Problem solving</u>***)

ABSORPTION AND EMISSION TECHNIQUES 4+1 hours

Quantitative aspects of spectrochemical measurements. Nephelometric and turbidimetric methods, choice of method and instrumentation. Analytical applications - turbidimetric titrations.

Quantitative aspects of fluorescence, fluorescence quantum yield. 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: interferences in AAS and corrections applied. ***Atomic emission method (AES), advantages and disadvantages,*** Plasma – ICP, ICP sources, DCP, and ICP-MS techniques.

FTIR SPECTROSCOPY **4+2 hours**

Infrared absorption process, uses of infrared spectrum. Bond properties and absorption trends. Instrumentation of IR spectrometer: Dispersive, Fourier transform spectrometers, ATR. Preparation of samples for IR analysis. ***Detailed discussions on C–H vibrations in sp, sp^2 and sp^3 hybridized carbon; difference between C=C and C≡C vibrations***; effects of conjugation, H-bonding, electron withdrawing groups, inductive, resonance, hydrogen bonding and conjugation on IR absorption. IR spectra of nitriles, isocyanates, isothiocyanates, and imines; nitro compounds; carboxylate salts, amine compounds and amino acids; sulfur compounds; alkyl and aryl halides; phosphorus compounds, metal-carbonyl complexes. Correlation charts and tables. Systematic analysis of an IR spectrum. ***IR analysis of simple molecules.***

^{1}H NMR SPECTROSCOPY **5 hours**

Coupling constants: The mechanism of coupling-one-bond couplings (^1J); two-bond couplings (^2J); three-bond couplings (^3J)-Karplus relationship. Long-range couplings (^4J–^nJ); magnetic equivalence. The 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.

C-13 NMR SPECTROSCOPY **6+1 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. ***Combined spectral problems***.

ADVANCED NMR TECHNIQUES **4+1 hours**

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

MASS SPECTROMETRY **7 hours**

Principle of mass spectrometry, mass spectrometer, resolution mass spectrum, molecular ion peak, base peak, fragment ion peaks, metastable 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 and amines. Different ionization and analysis methods: EI, CI, FAB, MALDI, etc. Structural determination of molecules.

REFERENCES

1. Fundamentals of Analytical Chemistry; D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch; 10th Edition, Cengage India Pvt. Ltd., 2023.
2. Principles of Instrumental Methods of Analysis; D. A. Skoog, F. J. Holler, S. R. Crouch, 7th Edition, Cengage India Pvt. Ltd., 2020.
3. Introduction to Spectroscopy; Donald L. Pavia, Gary M. Lampman, George S. Kriz and James R. Vyvyan; 5th Edition, Cengage Learning, 2019.
4. Organic Spectroscopy; William Kemp; 3rd Edition, Bloomsbury Publishing, 2022
5. Mass spectrometry: Principles and applications; de Hoffmann, E., and Stroobant, V.; 3rd Edition, Wiley, 2007.
6. Mass spectrometry: A textbook; Gross, J. H.; 3rd Edition, Springer, 2017.
7. Introduction To Spectroscopy, 5th Edition, Donald L. Pavia, Gary M. Lampman and George S. Kriz and James R. Vyvyan, Cengage Learning, 2015.
8. Analytical Chemistry; G. D. Christian, P. K. Dasgupta, K. V. Schug; Wiley India Pvt. Ltd., 2020.

Learning outcomes: After performing these experiments, students will be able to

LO1	Knowledge	Recall: significant figures and types of errors in chemical analysis, the principles of absorption and emission spectroscopy Define: spin-spin splitting, and coupling constants in ^{1}H and ^{13}C NMR spectroscopy.
LO2	Understand	Explain: the principle of chemical analysis and least-squares method, figures of merits in chemical analysis, different methods to minimize errors, principles of nephelometry and turbidimetry, coupling constants; stability trends of carbocations and fragmentation patterns in mass spectrometry; principles of 2D NMR and DEPT techniques in NMR spectroscopic analysis. Differentiate: between absorption and scattering techniques, between nephelometry and turbidimetry
LO3	Apply	Examine: different statistical tests to justify the authenticity of obtained results during chemical analysis Identify: functional groups using IR spectral data; chemical environment of the nuclei (^{1}H and ^{13}C) using chemical shift values. Determine: molecular weights and molecular formulae of organic compounds using *m/z* values in mass spectrometry. Compute: coupling constants from ^{1}H-NMR spectra.
LO4	Analyze	Analyze: the obtained data by subjecting them to different statistical treatments such as t-test, F-test, Q-test and Grubbs' test, absorption and emission spectra in terms of molecular structure and composition Examine: COSY 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.

LO5	Evaluate	Assess: the experimental data after performing hypothesis tests and decide whether to reject or accept the results obtained. Compare: the limitations and assumptions of absorption and emission techniques in various analytical applications Interpret: the splitting pattern in the ^{1}H NMR spectrum of a compound. Assess: the reliability and limitations of mass spectra techniques in structural determination of organic compounds.
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 Deduce: the molecular structure of unknown compounds using the combined spectral data.

Semester	**VII**
Paper code	**CHXXXX**
Paper title	**Chemistry Practical VII**
Number of teaching hrs per week	**3**
Total number of teaching hrs per semester	**33**
Number of credits	**2**

List of Experiments

1. Determination of statistical measures and functional relationships from multiple experimental data sets using the Least Squares Method (Non-Graphical Approach).
2. General characterization and identification of molecular functionalities of synthesized compounds /complexes using FTIR spectroscopy.
3. Quantitative and qualitative analysis of selected fluorescent compounds by fluorescent spectrophotometer.
4. To determine the turbidity of the given sample using nephelometer.
5. Estimation of sulphate concentration using turbidimeter.
6. Characterisation of synthesized compounds by UV-vis and FTIR and plotting the data using Origin Software.
7. Interpretation of ^{1}H-NMR, ^{13}C-NMR and mass spectral data of selected compounds (3 sessions).
8. Determination of Hammett acidity of some organic solvents.
9. Introduction to ChemDraw/ChemSketch: Drawing Structures, Practicing Reactions, and Exploring Functional Tools: A Practical approach.
10. Determination of acidity of solid acid catalysts using FTIR.
11. Repetition/viva.

REFERENCES

1. Principles of Instrumental Methods of Analysis, 7th Edn., D. A. Skoog, F. J. Holler, S. R.Crouch, Cengage India Pvt. Ltd., 2020.
2. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th Edition., Saunders College Publishing, USA, 2017.

3. Introduction to Spectroscopy, 5th Edn., D. L. Pavia, G. M. Lampman, G. S. Kriz, J. A. Vyvyan, Cengage Learning, 2014.
4. Fundamentals of Molecular Spectroscopy, 4th Edn., C. N. Banwell, E. M. McCash, McGraw Hill Education, 2017.
5. Organic Spectroscopy: Principles and Applications, 3rd Edn., Jag Mohan, Narosa Publishing House, 2016.

Learning Outcomes: After performing these experiments, students will be able to

LO1	Knowledge	Define mean, standard deviation, least squares fitting, turbidity and light scattering, Bronsted and Lewis acid sites, Hammett equation Recall typical IR absorption frequencies for functional groups, chemistry behind sulphate precipitation and turbidity, chemical shift ranges and common fragmentation patterns. List compounds that exhibit fluorescence.
LO2	Understand	Describe how molecular vibrations correlate with IR spectra. Explain the mechanism of fluorescence and its relation to molecular structure, nephelometric principles and their applications, the relevance of spectral features to compound structure, splitting patterns, coupling constants, and isotope peaks, symbolic representation of molecules and mechanisms. Discuss the relationship between turbidity and sulphate concentration. Describe how acidity affects reaction rates and equilibria.
LO3	Apply	Identify functional groups in compounds using FTIR spectra, chromophores involved in UV-Vis, software functions for drawing atoms, bonds, and reactions. Quantify and identify compounds using fluorescence data. Measure turbidity using appropriate instrumentation, absorbance or pKa in different solvent systems Prepare samples and standards for turbidimetric analysis. Assign peaks in NMR/mass spectra to specific structural elements. Apply ChemDraw or ChemSketch to draw structures and reactions.

LO4	Analyse	Interpret residuals and fitting accuracy, excitation/emission spectra for compound differentiation, absorbance peaks and assign structural features. Compare experimental spectra to reference data. Examine sample variations affecting turbidity readings. Analyze calibration data to determine unknown concentrations. Correlate spectral data with chemical structures. Calculate Hammett acidity function (H_0) from experimental data. Differentiate FTIR signatures of Brønsted vs. Lewis acids. Recognize errors in drawn structures or resonance forms.
LO5	Create	Propose a complete FTIR-based identification workflow for unknowns, modifications to enhance acidity or selectivity Design a fluorescence-based sensor for a given analyte, professional-quality reaction schemes for lab reports or publications Develop an optimized method for sulphate estimation in field samples. Generate comparative plots and summary reports using ORIGIN Construct a detailed structural proposal based on combined spectral data. Formulate hypotheses on solvent effects in acid-catalyzed reactions.
LO6	Evaluate	Evaluate spectral clarity and possible interferences. Interpret excitation/emission spectra for compound differentiation. Assess instrument calibration and sample preparation methods, spectral data quality and synthesis success, appropriateness of linear models for data sets Compare results with expected values and other methods, spectra of related compounds to infer structural variations, solvent acidities and their effects on chemical reactivity, different drawing tools and layouts for clarity and accuracy.

Semester	**VII**
Paper code	**CH XXX**
Paper title	**ADVANCED ORGANIC CHEMISTRY**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

STRUCTURE, REACTIVITY AND REACTION MECHANISMS 7+1 hours

(Resonance, field effects, hyperconjugation, steric effects), steric inhibition of resonance.

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

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

Reactive intermediates: Generation, structure, stability and reactivity of carbenes and nitrenes.

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

ADVANCED STEREOCHEMISTRY 7+1 hours

Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes, trans-cyclooctenes. Stereochemistry of catenanes, rotaxanes, knots and Mobius strips, cycloenantiomerism. Helicity – helicenes, P-M notations. ***In-out isomerism***. 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.

PERICYCLIC REACTIONS **14+2 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-Möbius (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.*** [2+2] addition of ketenes, 1,3-dipolar cycloadditions: ***application in click chemistry and bio-orthogonal chemistry***. Cheletropic reactions involving CO and SO_2.

Sigmatropic rearrangements: Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5-, 3,3- and 5,5-sigmatropic rearrangements; Cope, oxy-Cope and Claisen rearrangements. ***[3,3]-Sigmatropic rearrangement in Fischer Indole synthesis.*** Benzidine rearrangement.

Group transfer reactions: Alder-ene reaction.

Application of pericyclic reactions in Vitamin-D synthesis.

PHOTOCHEMISTRY **5+1 hours**

Photochemical reactions: Norrish type I and type II cleavages, cis-trans isomerization of stilbene, di-π-methane rearrangement; Paternò-Büchi reaction; photoreduction of ketones; ***photochemical oxidations: photosensitization oxidation and photosensitized oxygen transfer***, cycloaddition of singlet molecular oxygen. Photodynamic therapy. Photochemistry of arenes.

REARRANGEMENT REACTIONS **6+1 hours**

Carbon to carbon migrations: Wagner-Meerwein, pinacol-pinacolone, benzil-benzilic acid, Favorskii rearrangements; Arndt-Eistert synthesis; expansion and contraction of rings. Carbon to nitrogen migrations: Hofmann, Curtius, Schmidt and Beckmann rearrangements. Nitrogen/oxygen/sulfur to carbon migrations: Stevens and Wittig rearrangements.

Carbon to oxygen migrations: ***Baeyer-Villiger rearrangement.***

REFERENCES

1. Molecular orbitals and Organic chemical reactions, Ian Fleming, John Wiley, 1st Edition, 2010.

2. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory, S. Sankararaman, Wiley VCH, (2005).

3. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, 6th Edition. New Age International Publishers, 2024.

4. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy and J.C. Scaiano, University Science Books, 2010.

5. Pericyclic Reactions, S. Kumar, V. Kumar, and S. P. Singh, Academic Press, 2016.

6. Organic Photochemistry, J.M. Coxon and B. Halton, Cambridge India, 2nd Edn, 2015.

7. Modern Physical Organic Chemistry, E. W. Anslyn and D. Dougherty, University Science Books, U.S., 2006.

8. Photochemistry of Organic Compounds, Petr Klan and J. Wirz, 1st Edition, John Wiley and Sons Ltd., 2009.

9. Essentials of Pericyclic and Photochemical Reactions, Biswanath Dinda, 1st Edition, Springer, 2017.

10. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley and Sons, 2016.

11. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 5th Edition., New Age International Publishers, 2022.

12. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, 11th Edition., New Age International Publishers, 2022.

13. March's Advanced Organic Chemistry, Michael B. Smith and J. March, 6th Edition., John Wiley, 2007.
14. Advanced Organic Chemistry, Part A and B, F. A. Carey and J. Sundberg, 5th Edition., Plenum press, 2007.
15. Organic Chemistry, Paula Yurkanis Bruice, 8th Edition., Pearson Education, Inc., 2020.
16. Organic Chemistry, J. Clayden, N. Greeves, S. Warren , 2nd Edition., Oxford University Press, 2012.
17. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry and Kathleen S. Richardson, Pearson, 3rd Edition, 1997.

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

LO1	Knowledge	Define steric inhibition of resonance, axial chirality and provide examples, planar chirality and provide examples, helicity, in-out isomerism, HOMO, LUMO, bonding, antibonding, and nonbonding molecular orbitals Recall the Hammett and Taft equations, rules for nomenclature of bridged ring systems, the different classifications of pericyclic reactions, key features of cis-trans isomerization of stilbene and di-pi-methane rearrangement State the Hammond postulate and the Curtin-Hammett principle, the Woodward-Hoffmann rules for pericyclic reactions. List the characteristics of reactive intermediates such as carbenes and nitrenes, the molecular orbitals of ethylene, 1,3-butadiene, and 1,3,5-hexatriene, the examples of 1,3-dipolar cycloadditions, examples of carbon-to-carbon, carbon-to-nitrogen, nitrogen/oxygen/sulfur-to-carbon, and carbon-to-oxygen rearrangements.

		Name methods used for determining reaction mechanisms, components of a Diels-Alder reaction, examples of Norrish type I and type II cleavages
LO2	Understand	Explain the quantitative treatment of field and resonance effects using the Hammett and Taft equations, the basic concepts of thermodynamics and kinetics of reactions, Hammond postulate and its implications, Curtin-Hammett principle, how characterization of intermediates, kinetics, stereochemistry, kinetic isotopic effects, isotopic labeling experiments, and solvent effects can be used to determine reaction mechanisms. the origin of axial chirality in allenes, spiranes, and biphenyls, the origin of helicity in helicenes, the nomenclature system for bridged ring systems, the concept of molecular orbital symmetry, the Alder Endo rule, the rearrangement reactions and their mechanisms. Differentiate between thermodynamic and kinetic control in reaction, between conrotatory and disrotatory modes in electrocyclic reactions. Describe the generation, structure, stability, and reactivity of carbenes and nitrenes, the frontier orbitals of different systems, the structural features of fused and bridged ring systems, the mechanism of the di-pi-methane rearrangement, Paterno-Buchi reaction, photoreduction of ketones, the expansion and contraction of rings via rearrangement reactions. Illustrate the structures of decalins, norbornanes, and bicyclo[2.2.2]octane, the construction of Woodward-Hoffmann orbital Symmetry Correlation Diagrams for simple pericyclic reactions, the

		mechanisms of various photochemical reactions, the mechanisms of Hofmann, Curtius, Schmidt, and Beckmann rearrangements, the mechanisms of Wagner-Meerwein, pinacol-pinacolone, benzil-benzilic acid and Favorskii, rearrangements.
LO3	Apply	Predict the effect of substituents on reaction rates and equilibria using Hammett and Taft equations, the structure of the transition state of a reaction using the Hammond postulate, product(s) of given 1,3-dipolar cycloadditions, product of a given Cope, oxy-Cope, or Claisen rearrangement, the products of given Wagner-Meerwein, pinacol-pinacolone, benzil-benzilic acid and Favorskii rearrangements, the products of ring expansion and contraction reactions, Hofmann, Curtius, Schmidt, Beckmann, Stevens, Wittig and Baeyer-Villiger rearrangements. Interpret kinetic data to gain insights into reaction mechanisms. Assign R and S configurations to given axially chiral molecules, P and M notations to given planar chiral molecules. Draw the structures of helicenes with specified helicity, the structures of given bridged ring systems based on their name. Determine whether a given cycloaddition reaction is thermally or photochemically allowed based on orbital symmetry considerations.

LO4	Analyse	Interpret Hammett and Taft plots to understand the electronic effects of substituents. Deduce the mechanism of a reaction based on experimental evidence such as kinetics and stereochemistry, the mechanism of an unknown pericyclic reaction based on experimental data. Analyze the stability and reactivity of carbenes and nitrenes, the structural features that lead to axial, planar, and helical chirality, the role of orbital overlap in determining the feasibility and stereochemistry of pericyclic reactions, the driving forces and stereochemical outcomes of different rearrangement reactions. Compare and contrast the different types of molecular chirality, the FMO approach and the Woodward-Hoffmann orbital Symmetry Correlation Diagram method for rationalizing pericyclic reactions. Normal and inverse electron demand Diels-Alder reactions, the mechanisms of different photochemical reactions, the mechanisms of different carbon-to-carbon, carbon-to-nitrogen, etc., rearrangements. Determine whether a given molecule is chiral based on its structural features, the efficiency of a photochemical reaction based on its quantum yield, the type of rearrangement occurring in a given reaction based on the starting material and product.
LO5	Evaluate	Assess the validity of proposed reaction mechanisms based on experimental data, the stereochemical properties of complex organic molecules, the feasibility of a proposed pericyclic reaction based on orbital symmetry rules, the feasibility of using photochemical reactions for a

		given organic transformation, the synthetic utility of different rearrangement reactions. Evaluate different synthetic strategies involving pericyclic reactions for their efficiency and selectivity. Choose appropriate rearrangement reactions for specific synthetic transformations.
LO6	Create	Design experiments to elucidate the mechanism of an unknown organic reaction, molecules exhibiting specific types of chirality (axial, planar, helical), a synthetic route to a target molecule utilizing one or more pericyclic reactions, a photochemical synthesis of a target molecule, synthetic routes to target molecules utilizing various rearrangement reactions. Propose novel applications of pericyclic reactions in organic synthesis or related fields., a novel photochemical reaction for a specific transformation.

Semester	**VII**
Paper Code	**CHXXX**
Paper title	**Chemistry Practicals VII-II**
Number of Lab hours per week	**3**
Total number of Lab hours per semester	**33**
Number of Credits	**2**

List of experiments

I. Systematic analysis and identification of bifunctional organic compounds.

1. Model compound (1 Session)

2. Bifunctional compound 1 (1 Session)

3. Bifunctional compound 2 (1 Session)

4. Bifunctional compound 3 (1 Session)

5. Bifunctional compound 4 (1 Session)

II. Synthesis of organic compounds and characterization by FTIR

6. Synthesis of pinacolone by pinacol-pinacolone rearrangement (2 sessions)

7. Synthesis of benzilic acid by benzil-benzilic acid rearrangement (2 sessions)

8. Synthesis of benzanilide by Beckmann rearrangement (2 sessions)

9. Repetition/Viva-Voce/any other experiment

Total 12 sessions

REFERENCES

1. Laboratory Manual of Organic Chemistry; Day, Sitaraman and Govindachari; 5th Edition; Allied Publishers;1996.
2. Practical Organic Chemistry; Mannand Saunders; 4th Edition; Pearson India; 2009.
3. Textbook of Practical Organic Chemistry; A.I.Vogel; 5th Edition; Pearson Education Limited; 1996.

4. Textbook of Quantitative Organic Analysis; A.I.Vogel; 6th Edition; Pearson Education; 2009.
5. Laboratory Manual of Organic Chemistry; Raj.K.Bansal; 5th Revised Edition; New Age International Publishers; 2009.
6. Laboratory Manual of Organic Chemistry; Harry Linn Fisher; New Edition; Legare Street Press; 2023.

Learning Outcomes: After performing these experiments, the student should be able to:

LO1	Knowledge	Recall the principles, techniques, and systematic analysis procedures used in qualitative analysis of organic compounds 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 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	Explain the principles and procedures involved in qualitative analysis, including solubility due the presence of more than one functional group and chemical tests for identifying organic compounds Write the mechanisms of various organic reactions Visualize reaction set up under reflux, inert and other suitable conditions
LO3	Apply	Apply the change in solubility of the organic compound due the functional group, systematic analysis procedures and qualitative tests to effectively identify the functional groups present in the given organic compounds.

		Apply various oxidizing, reducing and other reagents to synthesize target organic molecule; spectroscopic methods (e.g., NMR, IR) to identify and confirm the homogeneity of the prepared organic compound
LO4	Analyse	Analyse the role of solvent in group classification of the organic compound and systematic analysis procedures in identifying the functional groups in the given bifunctional compound considering their advantages, limitations and trends in test results 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	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 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	Create innovative strategies, protocols, and frameworks for optimizing qualitative analysis procedures for organic compounds with multiple functional groups and systematic qualitative analysis of organic compounds Design alternate routes for the preparation of specific target molecules

Semester	**VII**
Paper code	
Paper title	**COORDINATION AND BIOINORGANIC CHEMISTRY**
Number of teaching hours per week	**3**
Total number of teaching hours per Semester	**45**
Number of credits	**3**

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

METAL – LIGAND BONDING 10+1 hours

Crystal field splitting in 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; 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).

STRUCTURE AND BONDING IN SELECTED METAL COMPLEXES 6 hours

Bonding in hydride, dihydrogen, isocyanide, mononuclear metal carbonyl, nitrosyl, and tertiary phosphine complexes, ligand cone angle in tertiary phosphine complexes.
Stereoisomerism – chirality, optical activity, Circular Dichroism, Optical Rotatory Dispersion, Cotton effect and absolute configurations.

ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 9+1 hours

Spectroscopic ground states, selection rules, term symbols for d^n ions, microstates, Racah parameters, Orgel and Tanabe-Sugano diagrams, spectra of 3d metal aqua complexes of trivalent V, Cr, Mn, Co, Ni and $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra, ***spectral behaviour of lanthanide ions.***

MAGNETIC PROPERTIES OF METAL COMPLEXES **6+2 hours**

Origin and types of magnetic behaviour; diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism. Magnetic susceptibility and its measurement by the Guoy 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, spin-only behaviour (explanation based on A, E and T terms) and spin-cross over.

Applications of magnetic data.

BIO-INORGANIC CHEMISTRY **8+2 hours**

Metal ion storage and transport: Ferritin, transferrin, ceruloplasmin, siderophores. (*Transport and storage of dioxygen: hemoglobin, myoglobin; phenomenon of cooperativity);* model systems (picket fence porphyrins), hemocyanin and hemerythrin. ***Transport of ions across membranes: Active and passive transport across the membrane***, ion transport, naturally occurring ionophores - ***antibiotics: eg: valinomycin and nonactin.*** Mechanism of ion transport: sodium potassium pump and Na^+/K^+ ATPase.

Metalloenzymes: Non-redox enzymes – ***carboxypeptidase A*** and carbonic anhydrase; redox enzymes - superoxide dismutase (***mono*** and binuclear), alcohol dehydrogenase.

REFERENCES

1. Inorganic Chemistry, 5th Edn., C. E. Housecraft and A. G. Sharpe, Pearson Education Ltd., 2018.
2. Inorganic Chemistry, 7th Edn., M. Weller, J. Rourke, T. Overton and F. Armstrong, Oxford Univ. Press, 2018.
3. Advanced Inorganic Chemistry, 3rd Edn., F. A. Cotton and G. Wilkinson, Wiley Eastern limited, 1972.
4. Inorganic Chemistry, 5th Edn., J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Pearson Education Asia Pvt. Ltd., 2022.

5. Inorganic Chemistry, R. C. Maurya, De Gruyter Publishing House, 2021.
6. Inorganic Chemistry, 5th Edn., G. L. Miessler, P. J. Fischer, D. A. Tarr, Pearson Education Ltd., 2014.
7. Theoretical Inorganic Chemistry, M. C. Day and J. Selbin, East West Press, second edition, 2008.
8. Bioinorganic chemistry, Asim K. Das, Books and Allied publishers (P) Ltd., Kolkata, 2020
9. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, Viva Books Pvt. Ltd., 1998.
10. Bioorganic and Supramolecular Chemistry, P. S. Kalsi, J. P. Kalsi, and Ashu Chaudhary, New Age International Publishers, 2020.

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

LO1	Knowledge	Recall the terms, concepts, rules, theorems, classifications, orbital splitting patterns, and energy level diagrams pertaining to metal-ligand (M-L) bonding, spectral, and magnetic properties of metal complexes. Write limitations of crystal field theory, origin and types of magnetic behaviour, Curie and Curie-Weiss laws, term symbols for d^n ions and their significance in determining electronic configurations, selection rules governing electronic transitions in transition metal complexes. List the role of different metal ions in biological systems, including coordination chemistry, redox reactions.
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 Describe the 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, spin-only behaviour, spin-cross over, stereoisomerism, chirality, optical activity, CD, ORD, Cotton effect. Recognize the applications of the fundamental principles of inorganic chemistry to bioinorganic systems
LO3	Apply	Calculate 10 Dq and β values from Tanabe- Sugano diagrams, stabilization due to tetragonal distortion, octahedral site preference energy in spinels and OSSE in complexes, magnetic moments 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. Apply knowledge of bioinorganic chemistry principles to analyze and solve complex problems related to metal ions. Modify existing metal-based drugs for better selectivity.
LO4	Analyse	Predict the possibility of Jahn-Teller distortion in different d^n configurations, preference for octahedral/tetrahedral geometry in complexes, and spinel structures Compare the steric and electronic properties of phosphine ligands Compare and contrast modern theories of bonding in the interpretation of the structures and properties of metal complexes. Illustrate the mechanism of action of enzymes in catalyzing diverse biochemical reactions, such as carriers of electrons and functional groups.

		Examine the redox properties of metal ions in biological systems. Compare the efficacy of different types of metals in biomedical applications.
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. Assess the experimental data and scientific literature to judge the contribution of bioinorganic chemistry to our understanding of biochemical phenomena, and to identify emerging trends and unanswered questions in the field.
LO6	Create	Validate the structures of a given complexes from spectral data and magnetic studies. Propose suitable mechanism of action for enzymes. Design and propose innovative approaches for studying and manipulating metal-ion mediated biological processes. Integrate concepts of bioinorganic chemistry with techniques from other scientific disciplines to address complex biological challenges

Semester	**VII**
Paper code	
Paper title	**FORENSIC CHEMISTRY**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

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

INTRODUCTION TO FORENSIC SCIENCE 6+3 hours

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

Case study - Amanda Knox: A Flawed Case of Murder

Legal aspects of crime- Role of Investigator.

Case study - Dr. Coppolino's Deadly House Calls

Classification of crime scene evidence – physical and trace evidence. Collection, labelling, sealing and transportation of evidences.

Case study - Psychopathic serial killer, Raman Raghav

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

IDENTIFICATION AND ANALYSIS OF EVIDENCE FOUND AT THE CRIME SCENE 11+1 hours

Duties of first responder at crime scene, chain of custody, reconstruction of scene of crime. Recording data and writing report on crime scene. Introduction of different toxins/poisons commonly used and identified in forensic laboratories. Toxicological analysis – detection of alcohol in blood sample, chemical intoxication tests - breath testing for alcohol. A short overview of the mechanism by which these toxins act that result in death. Drugs: Illegal drugs (e.g., cannabis, cocaine, opium, morphine and heroin), detection and identification of drugs. Consequences of drug overdose.

Fire: Introduction to Fire & Arson, origin of fire, chemistry of fire and analysis of fire debris. Explosive and Explosion: scope & significance of explosive analysis in forensic science.

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

<u>Case study - Bruce McArthur: A Mountain of Physical Evidence</u>

ANALYTICAL METHODS IN FORENSIC CHEMISTRY 17 hours

Different light microscopy techniques and their application in forensic: bright field, dark field, phase contrast, polarized light. comparison, stereo-zoom and fluorescence microscopy techniques. Electron Microscopy: scanning electron microscopy (SEM), transmission electron microscopy (TEM), scanning-transmission electron microscopy (STEM), scanning tunnelling microscopy (STM) and atomic force microscopy (AFM). Sample preparation for chromatographic and spectroscopic techniques. Chromatographic methods - forensic applications of thin layer chromatography, gas chromatography and liquid chromatography. Spectroscopic methods - forensic applications of ultraviolet-visible spectroscopy, infrared spectroscopy, Mass spectrometry and isotope ratio mass spectrometer. X-ray diffraction (EDX, WDX and XRD). Colorimetric analysis of narcotics. Electrophoresis –forensic applications. Forensic photography- Basic principles and applications of photography in forensic science.

FINGERPRINT METHODS IN FORENSIC CHEMISTRY 5+2 hours

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

<u>Case study - Killer Twin: Ronald and Donald Smith</u>

<u>Case study - The Mayfield Affair</u>

REFERENCES

1. Fundamentals of Forensic Science; M.M. Houck; J. A Siegel; Acadamic Press, London, 2006.
2. Analytical Techniques in Forensic Science; R. Wolstenholme; S. Jickells; S. Forbes; 1st edition, John Wiley & Sons Ltd, 2021.

3. Scientific techniques in criminal investigation; R. Ramachandran; 2nd edition, Kamal Publishers, 2021.
4. Forensic Science Identification of Fingerprints; K. C. Johari; 1st edition, Asian Law House, 2018.
5. An Introduction to Forensic Science in Criminal Investigation; R. Krishnamurthy; CRC Press, Selective & Scientific Books, 2022.
6. Criminalistics: An Introduction to Forensic Science; R. Saferstein; 13th Edition, Pearson Education, 2021.
7. Crime Scene Evidence: A Guide to the Recovery and Collection of Physical Evidence; M. Byrd; CRC Press, Boca Raton, 2001.
8. A Handbook on Drug and Alcohol Abuse: The Biomedical Aspects; F. G. Holfmann; Adele Hofmann; Oxford University Press Inc., 1983
9. Forensic toxicology in, Introduction to Forensic Sciences; A. Poklis; 2nd Edition, W.G. Eckert (Ed.), CRC Press, Boca Raton, 1997.
10. The Practical Methodology of Forensic Photography; D. R. Redsicker; 2nd Edition, CRC Press, Boca Raton, 2001.
11. Detection and identification of designer drugs by nanoparticle-based NMR chemosensing, L. Gabrielli, D. Rosa-Gastaldo, M.-V. Salvia, S. Springhetti, F. Rastrelli; F. Mancin, Chem. Sci., 2018, 9, 4777–4784.
12. DNA Analysis by application of Pt nanoparticle electrochemical amplification with single label response, S. J. Kwon, A. J. Bard, J. Am. Chem. Soc. 2012, 134, 26, 10777–10779.

Learning Outcomes: At the end of the course the students will be able to learn:

LO1	Knowledge	Recall the key definitions, historical aspects, and scope of forensic science, the standard duties of first responders and the concept of chain of custody, the principles of various microscopy, chromatography, and spectroscopy techniques and the basic types and patterns of fingerprints.
LO2	Understand	Understand: the importance of code of conduct, types of crime scenes, and crime scene search methods. Various poisons, toxins, and illegal drugs commonly encountered in forensic cases. Explain: principles behind latent fingerprint development.
LO3	Apply	Apply: procedures for securing, isolating, and processing indoor and outdoor crime scenes, analytical methods in

		solving forensic problems, physical and chemical methods for detecting latent fingerprints.
LO4	Analyze	Analyze the case studies to identify investigative flaws and patterns in criminal behavior.
LO5	Evaluate	Evaluate the role of investigators and the impact of legal frameworks on crime scene management, the reliability and limitations of different analytical techniques, the reliability of fingerprint evidence in court.
LO6	Create	Create criminal profiles based on psychological and forensic evidence including lie detection results.

Semester	**VII**
Paper code	
Paper title	**Industrial Chemicals, Analysis, Energy and Environment**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

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

INDUSTRIAL METALLURGY AND ALLOYS 6+1 hours

Preparation and applications of metals (ferrous and non-ferrous) (any two examples each) and ultrapure metals for semiconductor technology (silicon and germanium) ***Classification and importance of alloys***, Specific properties of elements in alloys. Processes involved in steel manufacture - removal of silicon, decarbonization, demanganization, desulphurization, dephosphorisation. Surface treatment (argon treatment, heat treatment carburizing).

CHEMISTRY OF INDUSTRIAL CERAMICS AND CEMENTING MATERIALS 6+2 hours

Ceramics: ***Important clays and feldspar, ceramic, their types***. Manufacture of high technology ceramics and their applications. Characteristics and applications of superconducting and semiconducting oxides (Two examples in each case). Structure and applications of fullerenes, carbon nanotubes and carbon fibre. Cement: ***Introduction to lime, gypsum plaster & cement, History of cementing materials, Classification of cement***, Raw materials for Portland cement, Manufacturing processes of cement. Influences of minor constituents, chemical analysis & quality control of Portland cement. Special cement- white cement, high alumina cement, rapid hardening cement, low heat cement, sulphate resisting cement and expansive cement.

SURFACE COATINGS & MODIFICATIONS 8 hours

Definition and significance of surface coating (e.g., corrosion resistance, wear protection, aesthetics). Types of coating: organic (paints, varnishes, polymers), inorganic (alumina, zirconia), metallic (electroplating, thermal spray). Applications. Case study: compare coatings for marine (saltwater corrosion) vs. biomedical (biocompatibility) applications.

Surface modification techniques: mechanical (shot peening, polishing), chemical (passivation, acid etching), thermal (laser treatment), plasma-based (plasma nitriding, PVD/CVD (physical/chemical vapor deposition).

Characterization & testing techniques: microscopy (SEM, AFM), adhesion tests (scratch, tape test), corrosion testing (salt spray, electrochemical). **Activity**: Analyze SEM images of coated vs. uncoated surfaces.

INDUSTRIALLY IMPORTANT CHEMICALS AND SAFETY DATA SHEETS 6 hours

Manufacture, application and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate. Industrial hazards and safety: Process hazards checklists, hazard surveys, safety program and Hazop safety reviews.

INDUSTRIAL CHEMICAL ANALYSIS AND SAMPLING 6+1 hours

Sampling procedures, sampling of bulk materials, techniques of sampling – solids, liquid and gases. Collection and processing of data.

Chromatography: ***Classification, principle and efficiency of the technique.*** Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal and elution method. Qualitative and quantitative aspects of chromatographic methods of analysis: TLC and HPLC. (spectral analysis of the given sample). Instrumental methods of analysis: Flame photometry, X-ray fluorescence, thermo-gravimetry. (basic concepts and instrumentations).

INDUSTRIAL POLLUTANTS, WASTE MANAGEMENT AND ENVIRONMENT

7+2 hours

Air Pollution: ***Major sources of air pollution. Effects of air pollution on living organisms and vegetation.*** Pollution by SO_2, CO_2, CO, NOx, H_2S and other foul-smelling gases. Methods of estimation of CO, NOx, SOx and control procedures.

Water pollution: ***Water resources, aquatic ecosystems, sources and nature of water pollutants, impacts of water pollution on hydrological and ecosystems.*** Hydrological cycle, water analysis: physical and chemical methods. Industrial effluents and their treatment (primary, secondary and tertiary). Sludge disposal, industrial waste management and incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis and ion-exchange).

REFERENCES:

1. Industrial Chemistry; B. K. Sharma; Goel Publishing House, Meerut, 2016.
2. Engineering Chemistry; P. C. Jain, M. Jain; Dhanpat Rai & Sons, Delhi, 2015.
3. Engineering Chemistry; R. Gopalan, D. Venkappayya, S. Nagarajan; Vikas Publications, New Delhi, 2013.
4. Fundamentals of Analytical Chemistry; Skoog, Douglas A., West, Donald M., Holler, James and Crouch, Stanley; 9th Edition, 2013.
5. Industrial Inorganic Chemistry; K.H. Buchel, Wiley-VCH, 2000.
6. Riegel's Handbook of Industrial Chemistry; J. A. Kent; CBS Publishers, New Delhi, 1997.
7. Principles of Environmental Engineering & Science; M. Davis, S. Masten; 3rd Edition, publication by McGraw-Hill, 2013.
8. Environmental Science; G. T. Miller, S. Spoolman;16th edition, 2019.
9. Industrial Water Pollution Control; W. Wesley Eckenfelder; 3rd edition, publishing by McGraw-Hill, 2000.
10. Wastewater Engineering: Treatment and Reuse; Metcalf & Eddy (Tchobanoglous, Burton, Stensel); 6th edition, publishing by McGraw-Hill, 2023.
11. Water Quality: An Introduction; C. E. Boyd: 2nd edition, publishing by Springer, 2020.
12. Surface Engineering for Corrosion and Wear Resistance; J.R. Davis: 1st edition, publishing by ASM International, 2001.

13. Handbook of Deposition Technologies for Films and Coatings; R. F. Bunshah; 3rd edition, publishing by Elsevier, 2010.
14. Introduction to Surface Engineering and Functionally Engineered Materials; Peter Martin; 1st edition, publishing by Wiley-Scrivener, 2011.

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

LO1	Knowledge	Identify and describe the composition and role of important raw materials used in ceramics and cementing materials. Identify the types of metals & alloys based on nature and composition and types of air & water pollutants. Classify different types of ceramics and cement based on their structure and applications, types of surface coatings based on material composition & applications and types of treatment of water based on nature of effluent. Describe the structure and components of an effective industrial safety program.
LO2	Understand	Describe the structure, properties, and uses of superconducting and semiconducting oxides with suitable examples. Explain the methods of preparation and applications of industrial important chemicals. Explain the procedure for the synthesis of metals & ultrapure metals. Discuss the methods of estimation of CO, NOx, Sox, greenhouse effect, ozone layer and global warming. Explain the importance and objectives of sampling in chemical and industrial analysis. Describe the principles, setup, and operational procedure of TLC and HPLC.
LO3	Apply	Identify and evaluate the physical and chemical hazards associated with the handling and storage of each listed chemical. Apply techniques for organizing, validating, and processing experimental or industrial data obtained from samples.

		Apply HPLC for quantitative analysis and interpret output data such as retention times and peak areas. Apply the methods of analysis and purification of water by various techniques. Apply various surface treatment methods to improve the quality of metals and alloys. Apply various techniques to modify the quality of surface coatings. Apply the methods of industrial waste management, slude disposal and incineration of waste.
LO4	Analyze	Analyze the effects of minor constituents on the properties and performance of cement. Interpret chemical analysis results and quality control parameters of Portland cement. Interpret safety data sheets (SDS) and apply standard safety precautions during the use and transport of hazardous chemicals. Interpret chromatographic data and report results in a scientifically accurate format. Analye the quality of water sample before and after treatment/ purification. Interpret the quality of metals, alloys and surface coatings before and after modifications.
LO5	Evaluate	Differentiate between special types of cement and explain their specific applications and advantages. Differentiate between primary, secondary and tertiary methods of treatment and compare the quality of purified water. Differentiate between various surface modified techniques to compare the quality of coatings and to be used for different applications.
LO6	Create	Create a method to dispose the industrial waste based on its origin. Create a method to purify the water/ air effluent based on its nature.

Semester	**VII**
Paper Code	**XXXX**
Paper title	**SUPRAMOLECULAR CHEMISTRY**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

INTRODUCTION TO SUPRAMOLECULAR CHEMISTRY 4+1 hours

Definition and historical development of supramolecular chemistry. Concepts of Host-guest chemistry, molecular recognition, and self-assembly. Differences between supramolecular and molecular chemistry. ***Examples of supramolecular systems in nature (e.g., enzymes, DNA).***

NON-COVALENT INTERACTIONS IN SUPRAMOLECULAR SYSTEMS 7+1 Hours

Hydrogen bonding: Principles, importance in biological systems, and design of synthetic systems. π-π interactions: Aromatic stacking, applications in molecular recognition. Van der Waals forces: Dispersion forces, their role in molecular aggregation. Electrostatic interactions: Ion-dipole and ion-ion interactions, salt bridges. Metal coordination: Role of metal-ligand interactions in supramolecular chemistry. Hydrophobic effects: Importance in self-assembly processes.

MOLECULAR RECOGNITION 9+1 hours

Principles of host-guest chemistry. Selectivity and specificity: Factors affecting recognition (size, shape, charge). Thermodynamics and kinetics of molecular recognition. Synthesis of macrocycles (cryptands, cyclam, calixarenes), thermodynamic and kinetic template effects. Macrocyclic effects and stability, crown ethers and lariat crown ethers.

Anion or cation binding: Concepts in anion or cation host design, different types of anion and cation hosts. Simultaneous cation and anion binding. Applications in sensors, catalysis, and drug delivery.

SUPRAMOLECULAR SYNTHONS AND CRYSTAL ENGINEERING 8+1 hours

Definition of supramolecular synthons, difference between homosynthons and heterosynthons, role of synthons in crystal engineering. ***The Cambridge structural database***, crystal engineering with hydrogen bonds, π-interactions - halogen bonding and other weak interactions, co-crystals, salts, polymorphs and their physico-chemical properties.

SUPRAMOLECULAR SELF-ASSEMBLY 11+2 hours

Mechanisms of self-assembly in biological and synthetic systems. Amphiphiles and micelles: Supramolecular chemistry of surfactants. Liquid crystals: Structure and properties of thermotropic and lyotropic systems. Supramolecular polymers: Dynamic assembly of polymers *via* non-covalent interactions. Coordination polymers and networks: Design and properties of metal-organic frameworks (MOFs). Soft matter systems: Hydrogels, vesicles, and their applications.

REFERENCES:

1. Supramolecular Chemistry; J. W. Steed and J. L. Atwood, 3rd Edition, John Wiley and Sons Ltd., 2022.
2. Core Concepts in supramolecular Chemistry and Nanochemistry; J. W. Steed, T. R. Turner and K. J. Wallace, John Wiley and Sons Ltd., 2007.
3. Supramolecular Chemistry; L. M. Lehn, VCH, 1995.
4. Crystal Design: Structure and Function; G. R. Desiraju, John Wiley and Sons Ltd., 2003.
5. Supramolecular Chemistry: An Introduction; V. F. John, John Wiley and Sons Ltd., 1993.
6. Supramolecular chemistry; P. D. Beer, P. A. Gale and D. K. Smith, Oxford university press, 1999.
7. Supramolecular Synthons in Crystal Engineering of Pharmaceutical Properties; A. K. Nangia, 1st Edition, Taylor and Francis Group, 2024.

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

LO1	Knowledge	Define supramolecular chemistry and describe its historical development. List the types of non-covalent interactions in supramolecular systems. Define host-guest chemistry and the principles of molecular recognition. Define supramolecular synthons and distinguish between homosynthons and heterosynthons. List the types of self-assembly processes in biological and synthetic systems.
LO2	Understand	Explain the concepts of host-guest chemistry, molecular recognition, and self-assembly. Explain the principles and importance of hydrogen bonding in biological systems. Explain factors affecting selectivity and specificity in molecular recognition (size, shape, charge). Describe the role of synthons in crystal engineering. Describe the structures and properties of amphiphiles, micelles, and liquid crystals.
LO3	Apply	Illustrate differences between supramolecular and molecular chemistry with examples. Demonstrate how π-π interactions facilitate molecular recognition. Calculate and interpret thermodynamic and kinetic parameters for host-guest systems. Use the Cambridge Structural Database to identify supramolecular synthons in crystal structures. Explain the formation of supramolecular polymers and coordination polymers.

LO4	Analyse	Compare supramolecular systems in nature (e.g., enzymes, DNA) to synthetic systems. Differentiate the roles of van der Waals forces, electrostatic interactions, and metal coordination in molecular aggregation. Compare different macrocycles (cryptands, cyclam, calixarenes) in terms of synthesis, stability, and recognition. Examine the impact of hydrogen bonding, π-interactions, and halogen bonding on crystal packing. Compare thermotropic and lyotropic liquid crystals in terms of structure and properties.
LO5	Evaluate	Assess the significance of supramolecular chemistry in biological and chemical contexts. Evaluate the role of hydrophobic effects in self-assembly processes. Assess the effectiveness of macrocyclic hosts for anion or cation binding in applications such as sensors and drug delivery. Assess the effects of co-crystals, salts, and polymorphs on the physico-chemical properties of materials. Evaluate the design and function of metal-organic frameworks (MOFs) in materials chemistry.
LO6	Create	Design a synthetic supramolecular system that utilizes specific non-covalent interactions. Propose a novel macrocyclic system tailored for simultaneous cation and anion binding. Design a co-crystal system using knowledge of supramolecular synthons. Design a soft matter system (e.g., hydrogel or vesicle) for a specific application (e.g., drug delivery or tissue engineering).

Semester	**VII**
Paper code	**CH XXXX**
Paper title	**RESEARCH METHODOLOGY**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

FUNDAMENTALS OF RESEARCH **9 + 1 hours**

What is Research? Objectives of research: theoretical models. Importance of methodology in scientific research: philosophy, concept, aim, purpose and scope of research. Types of research: descriptive vs analytical, pure vs applied, conceptual vs empirical, qualitative vs quantitative, scientific vs technical, diagnostic, evaluation, action and experimental research.

Review of Literature: Importance of literature review in defining a problem, literature sources-primary and secondary, reviews, monographs, patents, research databases, web as a source, searching the web, identifying gap areas from literature and research database, ***development of working hypothesis. Writing a literature review report.***

PLANNING OF RESEARCH **8 + 1 hours**

The planning process, selection and identification of a problem for research, formulation of the selected problems, hypothesis formation, measurement, research design/plan. Statement of research problem, meaning; importance; sources; evaluating a research problem, objectives, design and execution of experiments, collection and interpretation of experimental data, arriving at conclusions. Experimental research and design: approximation of data, simulation and modelling. Good laboratory practices and safety measures. Sampling: types of sampling, questionnaire and observational methods of data collection. Reporting the results of research – style and format – title, abstract and the text, references, tables, figures, elucidations, quotations and footnote.

Case studies.

TOOLS AND TECHNIQUES IN RESEARCH 8 + 1 hours

Use of search engines for literature review and gap identification: google scholar, scopus, science direct, Scifinder, internet archive, arxiv, web of science, research rabbit, pubmed, ResearchGate and shodhganga. Use of common software such as microsoft word, microsoft excel, latex, matlab. Application of common software in chemistry: chemsketch, chemdraw, and origin. AI in chemistry: tools for automating tasks, providing authentic data, streamlining the research process: chatgpt, mendeley, Zotero, EndNote, Bibtex and citemaker.

Use of Mendeley/Zotero in a report writing.

SCIENTIFIC COMMUNICATION 7 + 2 hours

Introduction to writing report, thesis, review, research paper and monographs. Steps to write a research paper: title, abstract and keywords, introduction, materials and methods, results and discussion, conclusion, references, conflict of interest, acknowledgment, tables, figures, schemes and graphs, appendices, supplementary information and cover letter. General communication in magazines, newspapers, blogs for science outreach and public engagement. Seminar/conference/webinar presentation: oral and poster. Research proposals: writing and submission.

Writing articles, a research proposal to industrial and academic funding agencies, and preparing a poster.

RESEARCH PUBLICATION AND ETHICS 7 + 1 hours

Types of journals and publications- domain-based, university, private, individual, regional, society/association, open access journals, article processing charges. Indexing - indexing agencies (Scopus, Web of Science, Vidhwan, Orcid) and indexing parameters. Concept of impact factor of journals: SNIP, SJR, IPP, Cite Score, Research interest score, h-index, d-index, ***calculation of h-index***, i10-index, altmetric. Publication ethics - definition, introduction and importance, best practices/standards setting initiatives and guidelines, conflict of interest, publication misconduct, violation of publication ethics, examples of fraud from India and abroad. Plagiarism and similarity: use of plagiarism software like Turnitin, Urkund, DrillBit plagiarism detection software and other open-source tools. Brief introduction to IPR: Patent, copyright and trademark.

REFERENCES

1. Research methodology – Methods and techniques; C. R. Kothari; and G. Gaurav; New Age International Publishers, 2019.
2. Research Methodology: Methods & Techniques; S. K. Gupta; and R. Praneet; Kalyani Publishers, 2017.
3. Research methodology – A step-by-step guide for beginners; R. Kumar; 2nd Edition, Pearson Education, 2016.
4. Research methods for science; M. P. Marder; Cambridge University Press, 2011.
5. Research methodology – Methods and techniques; C. R. Kothari; Wiley Eastern Limited, 2004.
6. How do I write a scientific article? A personal perspective; G. Lippi; Annals of Translational Medicine, 5(20), 416, 2017.
7. Writing scientific research articles: Strategy and steps; M. Cargill; and P. O'Connor; 2nd Edition, John Wiley and Sons, 2013.
8. Ethics in research; I. Gregory; Viva Books Pvt. Ltd., 2005.
9. Case study research methods; B. Gillham; Viva Books Pvt. Ltd., 2005.
10. Predatory Journals: What the Researchers and Authors Should Know; A. Chandra; and S. Dasgupta; The American Journal of Medicine, 6(137), 2024.
11. Predatory journals and their effects on scientific research community; F. Habibzadeh; and A. M. Simundic; Biochemia Medica, 27(2), 270, 2017.
12. Origin 9.1 User Guide – OriginLab (https://www.originlab.com/doc/User-Guide).

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

LO1	Knowledge	Define research. Recall the steps involved in the research planning process.

		List objectives and types, various research databases and software tools used in scientific research, different types of journals and indexing systems.
LO2	Understand	Explain the philosophy, purpose, scope of research and the role of methodology, the utility of AI and software tools like Mendeley, Zotero, and BibTeX in research, the concept of impact factor, h-index, plagiarism, and publication ethics. Describe the process of hypothesis formulation and experimental design. Discuss the formats and styles of various scientific communications (thesis, review, poster, blogs).
LO3	Apply	Distinguish between various types of research (qualitative vs. quantitative, empirical vs. conceptual, etc.). Demonstrate the use of sampling methods and data collection tools (questionnaires, observations). Apply search engines and databases (e.g., Google Scholar, Scopus) to find and manage research articles, the utility of AI and software tools like Mendeley, Zotero, and BibTeX in research. Prepare abstracts, keywords, and structured outlines for papers and presentations, a literature review with appropriate citations and structure. Utilize plagiarism detection tools to assess the originality of a document. Determine the best experimental approaches, research proposals or written manuscripts for clarity and relevance.
LO4	Analyse	Identify the sections of a research paper, a report, gap areas from literature and formulate a working hypothesis, unethical practices in research publication with examples. Examine a research problem to formulate objectives and an actionable design.

		Compare different tools and software for literature review and data analysis. Differentiate between scientific writing for academic and public audiences.
LO5	Evaluate	Assess the relevance and reliability of primary and secondary literature sources, research problems critically. Judge the effectiveness of specific digital tools in streamlining the research process. Evaluate the credibility of journals based on indexing and impact metrics.
LO6	Create	Design a detailed research plan, including problem statement, methodology, and expected outcomes. Compile references and citations using software tools in a well-structured research report. Write a complete research article or research proposal, and design a scientific poster. Draft an ethically sound publication-ready manuscript or patent application outline.

QUESTION PAPER PATTERN-END SEM EXAM (ESE)

St Joseph's University, Bengaluru-27

B.Sc. End Semester Examination

(2024-25 onwards)

CHEMISTRY

Time: 2 hours **Max. Marks: 60**

Instructions

1. The question paper has three Parts. Answer all the Parts.

2. Write chemical equations and diagrams wherever necessary.

PART– A

Answer any **SEVEN** of the following NINE questions. Each question carries **TWO** marks.

(7 x 2 =14)

PART– B

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

(6 x 6 = 36)

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 the mid-semester examination.

QUESTION PAPER PATTERN- MID SEM EXAM (MSE)

St Joseph's University, Bengaluru-27

B.Sc. Mid Semester Examination

(2024-25 onwards)

CHEMISTRY

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

Instructions

1. The question paper has three Parts. Answer all the Parts.
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 **TWO** of the following THREE questions. Each question carries **SIX** marks.

(2 x 6 = 12)

PART– C

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

(1 x 5= 5)

<u>**EVALUATION PATTERN - PRACTICALS**</u>

	Weightage in Marks
Formative Assessment (Internal assessment) Practicals	**30 (20 CIA + 10 Viva-voce)**
End semester practical examination (ESPE)	**20**
Total	**50**