ST JOSEPH'S UNIVERSITY
Bengaluru-27

Syllabus for

B.Sc.Chemistry

I-IV Semesters

2024-26

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. degree course is a three-year program divided into six semesters. Each semester will consist of 14 weeks of instruction for theory and 11 weeks of instruction for practicals. In Chemistry there will be 10 discipline core papers and 10 practical papers from I to VI 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 CH1P24	Chemistry I Practical I	45 44	**3** **3**	**40** **30**	**60** **20**	**100** **50**
II	CH224 CH2P24	Chemistry II Practical II	45 44	**3** **3**	**40** **30**	**60** **20**	**100** **50**
III	CH325 CH3P25	Chemistry III Practical III	45 44	**3** **3**	**40** **30**	**60** **20**	**100** **50**
IV	CH425 CH4P25	Chemistry IV Practical IV	45 44	**3** **3**	**40** **30**	**60** **20**	**100** **50**
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	45 44 45 44 45 44	**3** **3** **3** **3** **3** **3**	**40** **30** **40** **30** **40** **30**	**60** **20** **60** **20** **60** **20**	**100** **50** **100** **50** **100** **50**
VI	CH6126 CH6P1 CH6226 CH6P2 CH6326 CH6P3	Chemistry VI-1 Practical VI-1 Chemistry VI-2 Practical VI-2 Chemistry VI-3 Practical VI-3	45 44 45 44 45 44	**3** **3** **3** **3** **3** **3**	**40** **30** **40** **30** **40** **30**	**40** **30** **40** **30** **40** **30**	**100** **50** **100** **50** **100** **50**

Summary of credits for I-VI 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 CH6226 CH6P2 CH6326 CH6P3	Chemistry VI-1 Practical VI-1 Chemistry VI-2 Practical VI-2 Chemistry VI-3 Practical VI-3	3 3 3 3 3 3	3 2 3 2 3 2

Name of the Degree Program	B.Sc.
Discipline Core	Chemistry
Total Credits for the Program	128

Assessment: Weightage for assessments (in percentage)

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

SEP Syllabus: B.Sc. Chemistry – 1st Semester

I SEMESTER THEORY (CH 124)

Semester	**I**
Paper code	**CH 124**
Paper title	**Chemistry I**
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.

ANALYTICAL CHEMISTRY **3 hours**

Errors and treatment of analytical data: Errors - determinate and Indeterminate errors, replicate and outlier data points. Precision and accuracy; ways of expressing accuracy - absolute error, relative error; minimization of errors. Statistical treatment of random errors; mean, median, range, standard deviation and variance.

STOICHIOMETRY **2+1 hours**

(Atomic mass, gram atomic mass, molar mass, formula mass)

Avogadro number, mole concept and chemical equations. Concept of limiting reagents.

PERIODIC TABLE **4+2 hours**

General electronic configurations of s, p, d and f block elements and position of elements in the long form of periodic table. Atomic radius: covalent, metallic and van der Waal's radii, ionic radii. Effective nuclear charge (qualitative treatment); periodic trends in atomic radii; comparison of ionic radii of isoelectronic ions. Ionisation energy and electron affinity – periodic trends; factors affecting ionisation energy and electron affinity, ***successive ionisation energies***. Electronegativity- Pauling scale (only final equation), calculation of electronegativity, ***periodic trends***.

ATOMIC STRUCTURE **12+2 hours**

(Historical development of atomic structure, failure of classical mechanics in the study of subatomic particles: Black body radiation, Photoelectric effect).

de Broglie relation and Heisenberg's uncertainty principle. Thought experiment to understand uncertainty principle. Introduction to the principles of quantum (wave) mechanics: Operators - definition, quantum mechanical operators for position, momentum and energy; eigen functions and eigen values.

Schrödinger equation; Born interpretation of wave function (significance of ψ^2); postulates of quantum mechanics. Quantum mechanical treatment of particle in one- dimensional box: Derivation of expressions for energy and normalized wave functions of a particle in 1D box; energy level diagram. Energy expression for a particle in 3D box (no derivation); degeneracy in a cubic box.

Qualitative explanation of the emergence of quantum numbers and their significance; radial and angular components of the wave functions; radial distribution functions of s and p orbitals.

Shapes of s, p and d orbitals. Polyelectron atoms: electron spin and spin quantum number, (n+l) rule, Pauli's exclusion principle, Aufbau principle, Hund's rule, electronic configuration of atoms (Z = 1 to 30).

Exchange energy, pairing energy, promotional energy; symmetric distribution of electrons in atomic orbitals; prediction of the stable electronic configuration in p and d orbitals.

CHEMICAL BONDING- I **10+2 hours**

Covalent bonding: octet rule, Lewis structures of molecules and ions (when provided with sequence of atoms), formal charge calculation for different atoms in molecules/ions. ***Deviation from octet rule***. Valence bond treatment of hydrogen molecule: qualitative discussion of wave functions, concept of resonance.

Molecular structure: bond length, bond angle, dihedral angle and molecular geometry. Overlapping of atomic orbitals, σ and π bonds.

Hybridisation: sp (BeF_2), sp^2 (BF_3), sp^3 (SiF_4, H_2O, NH_3), sp^3d (PCl_5), sp^3d^2 (SF_6); examples of inorganic molecules (AB_n and AB_nL_m type) with and without π-bonds.

VSEPR theory: application to AB_n and AB_nL_m type molecules/ions (A = s or p block element; $n \leq 7$).

Molecular orbital (MO) treatment of hydrogen molecule: linear combination of atomic orbitals, bonding and antibonding orbitals, energy level diagram. MO energy level diagram of homonuclear diatomic molecules and ions ($Z \leq 9$): bond order and magnetic behaviour of these molecules and ions, correlation of bond order with bond length and bond strength. MO energy level diagram of heteronuclear diatomic molecules – HF and CO.

Metallic bonding: band theory (qualitative), ***classification of solids into conductors, insulators and semiconductors based on band theory***.

INTRODUCTION TO ORGANIC CHEMISTRY- I **5+2 hours**

Structural formulae: Dash, condensed and bond-line formulae. IUPAC nomenclature of monofunctional and bifunctional organic compounds. ***Trivial names and structures of common organic compounds***. Resonance theory, curved arrows in resonance structures, rules for writing resonance structures, resonance contribution. ***Concept of hybridisation: sp^3, sp^2, sp;*** **the structure and bond lengths of methane, ethane, ethene and ethyne.**

Physical properties and molecular structures of organic compounds, ionic compounds: ion–ion forces, intermolecular forces (van der Waals forces), boiling points.

REFERENCES

1. Principles of Inorganic Chemistry; B. R. Puri; L. R. Sharma and K. C. Kalia; 33rd Edition, Vishal Publishing Co., 2020.
2. Concise Inorganic Chemistry; J. D. Lee; 5th Edition, John Wiley and Sons Ltd; 2014.
3. Chemistry; R. Chang: 10th Edition, McGraw Hill Education India; 2022.
4. Principles of Physical Chemistry; B. R. Puri; L. R. Sharma and M. B. Pathania, 48th Edition, Vishal Publishing Co., 2021.
5. Atkins' Physical Chemistry; P. Atkins and J. Paula; 11th Edition, Oxford University Press, 2018.
6. Physical Chemistry for Chemical and Biological Sciences: Raymond Chang; 1st Indian Edition, Viva Books Pvt. Ltd., 2015.
7. Organic Chemistry; Graham Solomons, C. Fryhle, S. Snyder, 12th Edition, Wiley, 2017.
8. Organic Chemistry; P. Y Bruice, 8th Edition, Pearson Education India, 2020.

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

LO1	Knowledge	**Recall** the concepts of atomic structure, periodic table of elements, chemical bonding in molecules, concepts of stoichiometry and list the types of hybridisations, VSEPR principles, MO theory fundamentals, types of errors, rules for writing electronic configuration, naming organic compounds. **Identify** the different types of orbital overlap: end-to-end (forming sigma bonds) and side-to-side, name the different blocks and families of elements, examples of molecules exhibiting each type of hybridization. **State** the basic principles of VSEPR theory **Define** key concepts in Molecular Orbital (MO) theory, the Octet Rule, bond length, bond angle, dihedral angle.
LO2	Understand	**Explain** the relationship between molecular structure and physical properties, concepts, laws concerning atoms, molecules, atomic structure, chemical bonding, periodic table, stoichiometry, hybridisation concepts, VSEPR theory, and MO theory. **Describe** the process of hybridisation and its significance in determining molecular geometry. **Illustrate** the energy level diagrams of homonuclear diatomic molecules/ions ($Z \leq 9$) and heteronuclear diatomic molecules – HF and CO. **Outline** the differences between conductors, semiconductors and insulators based on band theory.
LO3	Apply	**Apply** the bonding theories in predicting structure, bonding and magnetic properties of molecules, laws and relationships to real chemical systems and compute properties. IUPAC rules to name simple and complex organic compounds, draw Lewis structures for common ions, including polyatomic ions like NH_4^+, SO_4^{2-}, and NO_3^-, draw resonance structures for given molecules. **Calculate** formal charges for atoms within a molecule or ion, empirical and molecular formulas, **Predict** the shapes of molecules based on their hybridisation states, the behaviour of solids as conductors, semiconductors and insulators based on band theory

		Construct MO energy level diagrams for simple diatomic molecules like H_2. **Interpret** the bond order and magnetic behaviour of homonuclear diatomic molecules/ions ($Z \leq 9$) from molecular energy level diagrams. **Relate** bond order with bond length and bond strength.
LO4	Analyse	**Validate** the quality of analytical data using statistical methods **Compare** different resonance structures of a molecule or ion, using formal charges. Compare the molecular geometries of different molecules based on their hybridisation states. **Analyse** the influence of lone pairs versus bonding pairs on predicting molecular shape, the impact of functional groups on reactivity and properties, the effects of resonance on molecular stability and reactivity. **Evaluate** the bond length and magnetic properties of molecules/ ions based on bond order. **Examine** the chances of forming/ stability of a diatomic molecule/ion based on MOT.
LO5	Evaluate	**Predict** stable electronic configuration in p and d orbitals with the help of various energy terms **Construct** molecular shapes using hybridisation concepts for complex molecules and molecular energy level diagrams for homonuclear diatomic molecules/ions (Z: 10-16).
LO6	Create	**Place** hitherto unknown element in the periodic table and predict its physical and chemical properties. **Judge** the effectiveness and limitations of VSEPR and molecular orbital theories in explaining molecular structures and properties. **Justify** the formation of certain molecules like NO, that cannot be successfully explained by either the Lewis electron-pair approach or valence bond theory, on the basis of MOT. **Assess** the bond orders and stability of homonuclear diatomic molecules/ions (Z: 10-16).

I SEMESTER PRACTICALS (CH 1P1)

Semester	**I**
Paper code	**CH 1P1**
Paper title	**Chemistry Practical I**
Number of Lab hours per week	**3**
Total number of Lab hours per semester	**33**
Number of credits	**2**

List of Experiments

1. Volumetric calibrations and statistical treatment of data.

2. Estimation of sodium hydroxide using hydrochloric acid.

3. Estimation of sodium hydroxide using potassium hydrogen phthalate.

4. Estimation of potassium permanganate using oxalic acid.

5. Estimation of iron (II) using potassium dichromate by internal indicator method.

6. Estimation of sodium carbonate and sodium bicarbonate in a given mixture.

7-10. RBPT experiments.

11. Demonstration of an auto-titrator during one of the RBPT sessions.

12. Viva/repetition.

Total 12 sessions

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

LO1	Knowledge	**Recall** the mole concept and define errors, accuracy, precision and significant figures. Calculate standard deviation and relate these to the concept of volumetric analysis. **Define** key terms related to volumetric titrations (e.g., titrant, analyte, equivalence point). **List** common indicators used in titrations.
LO2	Understand	**Compare** various ways of expressing concentration and explain the differences in them. **Explain** the principle and significance of volumetric titrations.
LO3	Apply	**Identify** the number of significant figures and solve numerical problems based on mole concept and chemical equations. **Calculate** the concentration of an unknown solution from titration data.
LO4	Analyse	**Apply** the theoretical concepts to develop experimental skills in carrying out volumetric analysis independently and draw inference/suggest a solution. Differentiate between types of titrations (e.g., acid-base, redox).
LO5	Create	**Propose** a research problem based on volumetric analysis, design an experiment and develop a method, discuss in a group and improvise the methodology, carryout independent work and create a personalized mode of presentation of results
LO6	Evaluate	**Assess** the accuracy and precision of titration results. Assess the errors in and calibrate the glassware used for experiments and estimate the amount of chemical substance present in a solution of unknown concentration.

<u>SEP Syllabus: B.Sc Chemistry – 2nd Semester</u>

II SEMESTER THEORY (CH 224)

Semester	**II**
Paper code	**CH 224**
Paper title	**Chemistry II**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

ACIDS, BASES AND SOLVENTS **5+1 hours**

Theories of acids and bases: Lowry - Brønsted concept, conjugate acid-base pairs, amphiprotic substances, relative strengths of acid-base pairs, solvent system concept of acids and bases, examples. Lewis concept - types of molecules or species that can act as Lewis acids and Lewis bases, Pearson's Hard and Soft Acid - Base concept. Characteristics of hard and soft acids and bases, HSAB principle and applications - stability of complexes, prediction of coordination in complexes of ambidentate ligands, predicting feasibility of a reaction, prediction of hardness and softness. Solvent properties - liquid range, dielectric constant, solvent polarity, classification of solvents. Protic solvents – autoionisation of protic solvents (H_2O, liq. NH_3). Aprotic solvents – classification with examples. Levelling effect of solvents - explanation, levelling solvents and differentiating solvents. Liquid NH_3 - autoionisation, acid-base reactions, solvation, solvolysis (comparison with H_2O in each case)**.** ***<u>Solutions of alkali metals in liquid</u>***

ammonia. Advantages and disadvantages of liq. NH_3 solvent. Liquid SO_2 as solvent - autoionisation and acid base reactions. Anhydrous HF - autoionisation, acid-base reactions.

CHEMICAL BONDING - II **3+1 hours**

Ionic bonding - lattice energy, explanation of melting point of simple ionic solids based on lattice energy. Born - Lande equation (no derivation). Born-Haber cycle for NaCl, ***KBr, KI***, MgO, $CaCl_2$. Covalent character of ionic bonds - polarisation and polarizability, Fajan's rules. Partial ionic character of covalent bonds, calculation based on Pauling electronegativity concept, dipole moment.

THE FIRST LAW OF THERMODYNAMICS **7+2 hours**

Introduction - terminology in thermodynamics - phase, system and surroundings. Types of systems - open, closed and isolated systems; homogeneous and heterogeneous systems, macroscopic properties. State of a system, state variable, extensive and intensive properties, thermodynamic equilibrium. Thermodynamic processes - isothermal, adiabatic, isochoric, isobaric and cyclic. Reversible, irreversible and spontaneous processes. Concept of heat and work, sign convention. State functions and path functions, exact and inexact differentials. Internal energy, first law of thermodynamics - statement and mathematical form. Enthalpy of a system, heat capacity, relation between C_p and C_v. Expression for first law of thermodynamics for isothermal, adiabatic, isochoric and cyclic processes. Work done in i) reversible expansion and compression, ***ii) irreversible isothermal expansion and compression of an ideal gas.*** Zeroth law and absolute temperature scale. Kirchoff's law-statement (no derivation).

GASEOUS STATE **3+1 hours**

The behaviour of real gases: Deviation from ideal gas behaviour. Compressibility factor (Z) and its variation with pressure for different gases. Causes of deviation from ideal behaviour, van der Waals equation of state (no derivation). Critical phenomena – Andrew's isotherms of CO_2, critical constants and their relation with van der Waals constant (no derivation). Joule-Thomson effect. Inversion temperature, application of Joule-Thomson effect.

LIQUID STATE AND LIQUID MIXTURES **5+1 hours**

Viscosity, coefficient of viscosity and surface tension of a liquid: definition. Variation of effect of temperature and solute in viscosity and surface tension of a liquid. ***Raoult's law, mathematical formulation***. Vapour pressure curves of ideal and type I solutions, non-ideal solutions and completely miscible liquids. Boiling point - composition curves of completely miscible liquids. Determination of molar mass using elevation in boiling point. Fractional distillation of binary liquid mixtures. Type II and Type III azeotropic mixtures (minimum boiling and maximum boiling azeotropes, e.g. water-ethanol and HCl-H_2O). Solubility of partially miscible liquid pairs; Critical solution temperature (CST), upper critical solution temperature (UCST): phenol-H_2O system, lower critical solution temperature (LCST): triethylamine-H_2O system; lower CST and upper CST: nicotine-H_2O system. Effect of impurity on CST. ***Immiscible liquid pairs: Nernst distribution law, effect of association and dissociation of solute on distribution (derivation).***

INTRODUCTION TO ORGANIC CHEMISTRY - II **6+2 hours**

Electronic displacements: Inductive effect, electromeric effect and hyperconjugation, (*resonance)*. Hückel's rule, aromatic, antiaromatic and nonaromatic species with examples. Strengths of organic acid and bases: Comparative study with emphasis on factors affecting pK_a values. Relative strength of aliphatic and aromatic carboxylic acids - acetic acid and chloroacetic acid, ***acetic acid and propionic acid, acetic acid and benzoic acid***. Relative strengths of ammonia, aliphatic and aromatic amines. Types of bond cleavages - homolytic and heterolytic cleavages; reaction intermediates - carbocations, carbanions and free radicals; generation, structure and stability. ***Types of reagents - electrophiles, nucleophiles.*** Types of organic reactions - substitution, addition, elimination and rearrangement: examples.

ALKANES AND CYCLOALKANES **7+1 hours**

Alkanes: Classification of carbon and hydrogen atoms in hydrocarbons. Physical properties of alkanes and cycloalkanes. Nomenclature of monocyclic cycloalkanes. Sigma bonds and bond rotation, meaning of conformations, Newman and Sawhorse projections. Conformational analysis of ethane and butane. Relative stabilities and ring strain of cyclopropane, cyclobutane and cyclopentane. Chair and boat conformations of cyclohexane and substituted cyclohexanes: axial and equatorial hydrogens. Conformational analysis of methyl cyclohexane, 1,3 - diaxial interactions of *tert*-butyl group.

REFERENCES

1. Principles of Inorganic Chemistry; B. R. Puri; L. R. Sharma and K. C. Kalia; 33rd Edition, Vishal Publishing Co., 2020.
2. Principles of Physical Chemistry; B. R. Puri; L. R. Sharma and M. S. Pathania, 48th Edition, Vishal Publishing Co., 2021.
3. Atkins' Physical Chemistry; P. Atkins and J. Paula; 11th Edition, Oxford University Press, 2018.
4. Chemical Thermodynamics: Classical, Statistical and Irreversible; J. Rajaram and J. C. Kuriacose; 1st Edition, Pearson Education India, 2013.
5. Physical Chemistry through Problems; S. K. Dogra and S. Dogra; 2nd Edition, New Age International (P) Ltd. Publishers, 2015.
6. Physical Chemistry for Chemical and Biological Sciences: R. Chang; 1st Indian Edition, Viva Books Pvt. Ltd., 2015.
7. Thermodynamics for Chemists, S.Glasstone, EWP, 2008.
8. Organic Chemistry; G. Solomons, C. Fryhle, S. Snyder, 12th Edition, Wiley, 2017.
9. Organic Chemistry; P. Bruice, 8th Edition, Pearson Education India, 2020.
10. Organic Chemistry; B. Mehta and M. Mehta, 2nd Edition, PHI Learning private limited, 2021.
11. Organic Chemistry; Jr. L. G. Wade, J. Simek, M Singh, 9th Edition, Pearson Education India, 2019.
12. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, 2nd Edition, Oxford University Press, 2014.

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

LO1	Knowledge	**Define** macroscopic properties, state variable, extensive and intensive properties, types of systems (open, closed, isolated), Inductive effect, electromeric effect, hyperconjugation, aromatic, antiaromatic and nonaromatic species with examples, homolytic and heterolytic cleavages; reaction intermediates- carbocations, carbanions and free radicals, electrophiles, nucleophiles, and conformations, Inversion temperature, lattice energy **Draw** the structures to represent Newmann and Sawhorse conformations of alkane and cycloalkane. **Recognize** and list the type of electronic displacements in organic molecules, cycloalkane from the nomenclature, the concept of ideal gases and real gases, meaning of ionic bonding **Draw** the structures to represent the electronic displacements, Newmann and Sawhorse conformations, draw resonance/canonical structures for the given molecule, Andrew's isotherms of CO_2, Born-Haber cycle for NaCl, MgO, $CaCl_2$ **State** HSAB principle, First law of thermodynamics, Zeroth law, Kirchoff's law, Raoult's law, Nernst Distribution law. van der Waals equation of state, Joule-Thomson effect, Born-Lande equation, Hückel's rule **List** the characteristics of hard and soft acids and bases, protic and aprotic solvents, the factors affecting the strengths of acids and bases, types of bond cleavage, types of organic reactions, classes of bonded hydrogen atoms, the criteria for the validity of Nernst distribution law, macroscopic properties of the system **Define** Lowry-Brønsted acids and bases, levelling effect of solvents, 'conformations' surface tension, viscosity, coefficient of viscosity, critical solution temperature **Recall** Raoult's law **Identify** Type I, Type II and Type III azeotropic mixtures, state variables

		Explain Type I azeotropic mixture, Type II azeotropic mixture, Type III azeotropic mixture, surface tension of a liquid, the effect of solute on the surface tension of a liquid, the effect of temperature on surface tension of a liquid, the effect of temperature on the viscosity of a liquid, the effect of solute on the viscosity of a liquid, the various thermodynamic processes: isothermal, adiabatic, isochoric and cyclic, the concept of heat and work with sign conventions, thermodynamic equilibrium, the relationship between C_p and C_v
LO2	Understand	**Discuss** the solvent system concept of acids and bases, thermodynamic processes, the factors influencing pK_a, the difference between Type I and Type II azeotropic mixtures; the difference between Type II and Type III azeotropic mixtures; the difference between Type I and Type III azeotropic mixtures; the difference between the lower CST and upper CST, causes of deviation of real gases from ideal behaviour, critical constants and their relation with van der Waals constant, applications of Joule-Thomson effect, explanation of melting point of simple ionic solids based on lattice energy **Describe** the relationship between the concentration of phenol in water and CST, the relationship between the concentration of nicotine in water and CST **Predict** the molecule as aromatic, antiaromatic or non-aromatic, predict the product of the reaction based on the type of organic reaction, variation of real gases with pressure **Classify** state functions and path functions, the types of solvents, the types of reactions, types of carbons and hydrogens **Interpret** the mechanism behind how the Type I, Type II and Type III azeotropic mixture plots vary with each other. **Compare** the properties of protic and aprotic solvents, the strengths of organic acids and bases, relative stability of conformations of alkanes and cycloalkanes, ideal and real gases based on their behaviour under different conditions, melting point of different ionic solids **Distinguish** reversible and irreversible processes, electrophiles and nucleophiles, axial and equatorial bonds,

		exact and inexact differentials, state function and path function, reversible and irreversible processes. **Understand** the relationship between size, shape, mass of molecules with the viscosity of the liquid, the relationship between temperature and viscosity, the relationship between temperature and surface tension **Outline** the concept of lower CST; upper CST; azeotropic mixtures
LO3	Application	**Apply** HSAB principle to predict the stability of complexes, Kirchoff's law to solve problems in thermodynamics, Hückel's rule to cyclic organic molecules, pK_a to order the strengths of acids and base, the data of surface tension values to understand the nature of the liquid the date of viscosity to understand the nature of the liquid, Joule-Thomson effect to different gases, Born-Lande equation to calculate lattice energy of different ionic solids zeroth law to find the absolute temperature scale **Examine** the correctness of electronic displacements and the resultant structures, the relationship between internal energy and enthalpy, the behaviour of different gases under variable pressure conditions **Sketch** the energy profile diagram of conformations of ethane, butane and cycloalkanes **Select** the hard and soft acids and bases from a given list, the electrophiles and nucleophiles from a list of reagents, the most acidic and basic compound, the most stable conformation of the given alkane and cyclohexane **Predict** the feasibility of a reaction using HSAB concept, the stable conformer in the presence of a bulky group, lattice energy of different ionic solids **Relate** C_p and C_v , the stability of cycloalkanes to ring strain, stability of conformations of cyclohexane to the presence of a bulky group and position of the group
LO4	Analysis	**Analyse** work done in irreversible expansion and compression of an ideal gas, reversible isothermal expansion and compression of an ideal gas. Acid-base reactions, the conformational analysis of ethane, butane and cyclohexane, the effect of the presence of bulky groups on the stability of the conformational structure, the deviation of real gases from

		ideal behaviour, total energy associated with formation of ionic solid based on Born-Haber cycle **Interpret** the nature of the azeotropic mixture by analysing a given plot
LO5	Create/Synthesis	**Construct** energy profile diagram of the given alkane, Andrew's isotherms of given gas, Born-Haber cycle for given ionic solid **Design** a reaction to obtain a certain intermediate for a product from a given compound. **Modify** the pK_a value of a given organic acid by fine tuning the substitutions
LO6	Evaluate	**Evaluate** the reasons for relative acid and base strength, stability of specific conformations of ethane, butane and substituted cyclohexane, the cause of deviation of real gases from ideal behaviour, melting point behaviour of different ionic solids, the effectiveness of the first law of thermodynamics in real world systems **Assess** the behaviour of an aromatic, anti-aromatic and a non-aromatic compound, steric hindrance by methyl and *t*-butyl groups, the behaviour of any gas under given conditions of temperature and pressure, accuracy of the thermodynamic calculations to experiments

II SEMESTER PRACTICALS (CH 2P1)

Semester	**II**
Paper code	**CH 2P1**
Paper title	**Chemistry Practical II**
Number of Lab hours per week	**3**
Total number of Lab hours per semester	**33**
Number of credits	**2**

List of experiments

1. Demonstration on mixing behavior of liquids and separation of liquids using their boiling points.
2. Determination of density using specific gravity bottle and viscosity of liquids using Ostwald's viscometer.
3. Determination of the density using specific gravity bottle and surface tension of liquids using stalagmometer.
4. Determination of partition/distribution coefficient of acetic acid in water and butanol.
5. Determination of composition of sucrose solution by viscosity method using Ostwald's viscometer.
6. Determination of CST of phenol- water system.
7. Determination of molar mass of an electrolyte by elevation in boiling point method.
8. Determination of percentage composition of sodium chloride solution by miscibility temperature measurements of phenol – water system.
9. Determination of transition temperature of a salt hydrate by thermometric method.
10. Recrystallisation of organic compounds and determination of purity by melting point.
11. Estimation of purity of aspirin.
12. Repetition/viva.

Total 12 sessions

REFERENCES

1. Principles of Physical Chemistry, B. R. Puri; L R Sharma and M. S. Pathania, 48^{th} Edition, Vishal Publishing Co., 2021.
2. Physical Chemistry laboratory manual: an interdisciplinary approach, A. Anand, R. Kumari, I. K. International Pvt Ltd.,2019.
3. Experiments in Physical Chemistry, C. W. Garland, J. W. Nibler, D. P. Shoemaker, 8^{th} Edition; McGraw-Hill: New York, 2003.
4. Experimental Physical Chemistry, A. M. Halpern, and G. C. McBane, 3^{rd} Edition; W.H. Freeman and Co.:New York, 2003.

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

Learning Objective	Cognitive Level	At the end of the semester, the student should be able to
LO1	Knowledge	**Define** surface tension, viscosity, coefficient of viscosity, critical solution temperature, partition coefficient **Recognize** the formation of homogeneous and heterogeneous mixtures, miscible and partially miscible liquids, the conditions under which Nernst distribution law is valid. **State** Nernst distribution law **Identify** the factors affecting the mixing of liquids , viscosity iii) surface tension, recystallisation of solids, CST, partition coefficient
LO2	Understand	**Discuss** the concept of miscibility and immiscibility in liquids, how impurities affect the boiling point of liquids, the difference between the lower CST and upper CST **Interpret** phase behaviour of the phenol-water system with varying concentrations of sodium chloride **Understand** method of using a stalagmometer to determine the surface tension of liquids the relationship between temperature and viscosity, the

		relationship between temperature and surface tension how to use a specific gravity bottle to measure the density of liquids accurately, the concept of partition coefficient, the concept of a) lower CST; b) upper CST, concept of transition temperature in salt hydrates , relationship between purity and melting point, phase transitions, concept of colligative properties
LO3	Application	**Examine** the composition of a solute in a solution using miscibility temperature measurements, behaviour and properties of binary mixtures, recrystallization conditions to maximize yield and purity **Sketch** temperature-composition graphs, temperature vs. time graphs to determine to determine the transition temperature, viscosity versus concentration graphs **Relate** partition coefficient distribution of a solute between two immiscible solvents, density of liquids with viscosity, miscibility and CST
LO4	Analysis	**Analyse** the relationship between density and viscosity in different liquids, factors affecting surface tension and its implications in various chemical processes , the phase behavior of the phenol-water system, the data to calculate the molar mass and understand its significance in solution chemistry, the thermal properties of salt hydrates and their applications, the effect of temperature on solubility of partially miscible liquids, how different solvents affect the recrystallization process
LO5	Create/Synthesis	**Develop** practical skills in performing distillation and analysing the purity of separated liquids skills in preparing and analysing a two-phase system, skills in using Ostwald's viscometer for compositional analysis skills in interpreting phase diagrams and miscibility data skills in recrystallization to purify compounds proficiency in analysing the purity of aspirin using titration methods
LO6	Evaluate	**Evaluate** partition coefficient and understand its relevance in extraction processes, how impurity affects CST, the practical applications of surface tension measurements in industries

SEP Syllabus: B.Sc. Chemistry – 3rd Semester

III SEMESTER THEORY (CH325)

Semester	**III**
Paper code	**CH325**
Paper title	**Chemistry III**
Number of teaching hours per week	**3**
Total number of teaching hours per semester	**45**
Number of credits	**3**

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

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

SECOND AND THIRD LAW OF THERMODYNAMICS 12 + 3 hours

Laws of thermodynamics - ***limitations of first law***, scope of second law, statement of second law. ***Spontaneous and non-spontaneous processes.*** Introduction to the concept of entropy. Heat engine; Carnot cycle – derivation of efficiency based on entropy concept. Entropy changes in adiabatic and isothermal reversible expansion of an ideal gas. Entropy of an ideal gas as a function of P, V and T. Entropy changes of an ideal gas for isothermal, isochoric and isobaric processes. Entropy of phase transitions. Entropy changes in the system and surroundings for reversible and irreversible processes. Entropy as a criterion for spontaneity. Physical significance of entropy. Entropy and spontaneity. Standard free energy change of a reaction. Free energy – Gibbs free energy and Helmholtz free energy. Gibbs free energy as a criterion of spontaneity. Relationship between work and work function (ΔA); work and change in Gibbs free energy (ΔG). Variation of G with T and P. Gibbs-Helmholtz equation. Van't Hoff's reaction isotherm. Clausius-Clapeyron equation – derivation, application to liquid-vapour and solid-liquid equilibria. Third law of thermodynamics – statement, the relationship between entropy and probability. Determination of absolute entropies of substances, standard entropies and residual entropy. ***Numericals. Case study: compare the thermodynamic aspects involved in the nuclear accidents: i) Fukushima accident and ii) Chernobyl accident; refrigeration cycle (or industrial boilers); and mixing of solutions***.

CHEMICAL KINETICS **4+1 hours**

(Review of chemical kinetics: definitions of rate of a reaction, order, molecularity, rate constant, rate equation or law, half-life, zero order and first order, pseudo-first-order reaction)

Derivation of rate expressions for a 2^{nd} order reaction when a=b and a≠b. ***Methods of calculation of order of a reaction i) integral and graphical method, ii) half-life period method***. Effect of temperature on reaction rates, temperature coefficient. Arrhenius theory, concept of energy barrier. Bimolecular collision theory [final equation given, no derivation], limitations of bimolecular collision theory. Transition state theory – qualitative approach. Steady-state approximation, Lindemann theory-kinetics of unimolecular reactions. Qualitative treatment of theory of absolute reaction rate.

Numericals. Case studies: catalytic converters and chymotrypsin, depletion of the ozone layer, Smog

CHEMISTRY OF REPRESENTATIVE ELEMENTS **8 + 2 hours**

(Periodic property of elements of alkali and alkaline earth metals with respect to electronic configuration, atomic and ionic radii, ionization energy, and electronegativity)

Chemistry of s-block elements: Oxidation state, melting point and boiling point, ***density, metallic character***, nature of bonds formed, diagonal relationship, and anomalous behaviour of the first member of each group. Oxides, peroxides, superoxides - formation, reaction with water, alkaline properties, basic character of oxides and hydroxides, flame coloration. Group I: photoelectric effect, Group II: comparison of solubilities of hydroxides and sulphates.

Chemistry of p-block elements: Inert pair effect, the relative stability of different oxidation states, metallic character, nature of bonds formed, alkaline properties, basic character of oxides and hydroxides, anomalous behavior of the first member of each group, allotropy, ***and catenation***.

Group 13: Structure of B_2H_6 - explanation of bonding based on VBT. Halides - comparison of Lewis acidic character of boron trihalides.

Group 14: Carbides – salt-like, covalent and interstitial. Silicates: classification, ortho, pyro, chain, sheet and three-dimensional silicates with examples. Zeolites: general formula, classification - natural and synthetic, ***applications.***

Group 15: Oxides and oxyacids of nitrogen and phosphorous –N_2O, NO, NO_2, N_2O_5, HNO_2, HNO_3, P_4O_6, P_4O_{10}, phosphoric and phosphorous acid series.

Group 16: Oxyacids and peroxoacids of sulphur – characteristics: sulphurous acid, sulphuric acid. Anomalous behaviour of oxygen.

STEREOCHEMISTRY **12 + 3 hours**

Constitutional isomerism and stereoisomerism: constitutional isomers, enantiomers, diastereomers and chiral molecules. Chirality and stereochemistry. Molecules having one chiral centre, test for chirality - plane of symmetry; R, S system of naming enantiomers. Properties of enantiomers: optical activity and its origin, specific rotation. Polarimeter experiment. Molecules with more than one chiral centre, meso compounds, Fischer projection formulae. Separation of enantiomers: resolution, examples of resolving agents. Chiral molecules that do not possess a chirality centre: diphenyls, allenes.

Diastereomerism: E, Z isomerism in alkenes, cis-trans isomerism in 1,2-dimethylcyclopropane,

Case studies of chiral drugs: R, S-ibuprofen, ***thalidomide, L- and D-cetirizine.***

End chapter problems.

REFERENCES

1. Principles of Inorganic Chemistry; B. R. Puri; L. R. Sharma and K. C. Kalia, 33rd Edition, Vishal Publishing Co., 2020.
2. Principles of Physical Chemistry; B. R. Puri; L R Sharma and M. B. Pathania, 48th Edition, Vishal Publishing Co., 2021.
3. Physical Chemistry; P. Atkins and J. Paula; 11th Edition, Oxford University Press, 2018.
4. Chemical Thermodynamics: Classical, Statistical and Irreversible; J. Rajaram and J. C. Kuriacose; 1st Edition, Pearson Education India, 2013.
5. Physical Chemistry through Problems; S. K. Dogra and S. Dogra, 2nd Edition, New Age International (P) Ltd. Publishers, 2015.

6. Physical Chemistry for Chemical and Biological Sciences: Raymond Chang; 1st Indian Edition, Viva Books Pvt. Ltd., 2015.
7. Organic Chemistry; T. W. G. Solomons, C. B. Fryhle and S. A. Snyder, 12th Edition, Wiley India, 2016.
8. Organic Chemistry; R. T. Morrison and R. N. Boyd, 7th Edition, Prentice Hall, 2010.
9. The Organic Chemistry of Drug Design and Drug Action; R. B. Silverman and M. W. Holladay, 3rd Edition, Elsevier Inc., 2015.
10. Foye's Principles of Medicinal Chemistry; D. A. Williams and T. L. Lemke, 7th Edition, Lippincott Williams & Wilkins, 2013.
11. Concise Inorganic Chemistry; J. D. Lee, 5th Edition, Blackwell Science, Oxford University Press, 2023.
12. Principles of Inorganic Chemistry; B. R. Puri, L. R. Sharma and K. C. Kalia, 33rd Edition, Vishal Publishing Co., 2020.
13. Inorganic Chemistry; Weller, Overtone, Rourke and Armstrong, 7th Edition, Oxford University Press, 2018.

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

LO1	**Knowledge**	**Define** entropy, List the limitations for of the first law of thermodynamics, state the second law of thermodynamics, second order reaction, temperature coefficient, energy barrier, threshold energy, energy of activation, effective collisions, collision number, collision frequency, steric factor, entropy, inert pair effect, allotropy, catenation, and oxidation states. Constitutional isomers, enantiomers, diastereomers, and chirality. Entropy, constitutional isomers, enantiomers, diastereomers, and chirality. **List** properties of p-block elements, the oxides and oxyacids of nitrogen and phosphorus, the limitations for first law of thermodynamics, the characteristics of optically active compounds **State** second law of thermodynamics, bimolecular collision theory, transition state theory. **Draw** an energy profile diagram for the formation of hydrogen iodide. Effective collisions, collision number,

		collision frequency, steric factor. **Explain** steady-state approximation **Identify** the types of carbides and classify silicates.
LO2	**Understand**	**Explain** the concept of entropy as a measure of disorder or randomness in a system and its role in thermodynamic processes, the characteristics of a second order reaction, the qualitative approach of transition state theory (activated complex theory), steady state approximation, Lindemann theory in the kinetics of unimolecular reactions, the differences between enantiomers and diastereomers, trends in oxidation states, melting/boiling points, density, and metallic character in s-block elements, the photoelectric effect in alkali metals, the bonding in diborane, the chemical behavior of selected oxides of nitrogen and phosphorous. **Derive** second order rate expression. **Describe** the concept of optical activity and how it is measured using a polarimeter, the formation and reactivity of oxides, peroxides, and superoxides with water, basicity trends of the oxides, peroxides and superoxides with water, the role of inert pair effects in stabilizing lower oxidation states, the anomalous behaviour of oxygen, the characteristics of sulfurous and sulfuric acids. **Differentiate** between salt-like, covalent, and interstitial carbides.
LO3	**Apply**	**Apply** the second law of thermodynamics to heat engine (Carnot cycle) and calculate efficiency using entropy concept. Calculate entropy changes for various processes, including isothermal, adiabatic, and reversible processes, the concept of axial chirality to identify chirality in allenes or

		biphenyls. **Calculate** the rate of a reaction, the rate constant, and the half-life of a second-order reaction, the order of a reaction using (i) integral and graphical method (ii) half- life period method. **Explain** bimolecular collision theory for a given reaction. **Assign** R or S configuration to a given chiral molecule. **Use** the plane of symmetry test to determine whether a molecule is chiral or achiral, trends in oxidation states to predict chemical reactions **Justify** the flame coloration in the group I and some of the group II elements **Ascertain** why the photoelectric effect is observed in alkali metals. **illustrate** examples of allotropy **Predict** the Lewis acidic character of boron trihalides in chemical reactions.
LO4	**Analyze**	**Analyze** the spontaneity of a reaction using Gibbs-Helmoltz equation, the importance of kinetic studies in the case studies: catalytic converters, chymotrypsin, depletion of the ozone layer, smog, the molecules with multiple chirality centers as meso compounds, **Compare** and contrast constitutional isomers and stereoisomers, the diagonal relationship and anomalous behavior of the first elements in groups I and II, the solubilities of hydroxides and sulfates of group II elements, the relative Lewis acidity of different boron halides, the oxidation states in oxides of nitrogen **Relate** inert pair effects and oxidation states of group 13

		and above elements
LO5	**Evaluate**	**Evaluating** the necessity of third law of thermodynamics. **Interpret** the kinetics of photochemistry in photosynthesis and photography, the kinetics of catalysis in industrial production, environmental safety, etc., whether a molecule exhibits chirality based on its structure and substituents. **Assess** the role of zeolites in industrial catalysis.
LO6	**Create**	**Assess** the role of chemical kinetics in the real world and evaluate the economic implications locally and globally. **Design and optimize** the practical processes, such as combustion, catalysis, battery technology, polymerization, and nanoparticle production based on chemical kinetics, the storing of drugs and pharmaceuticals to increase their shelf life based on chemical kinetics, the process of adding preservatives to food to prevent it from going bad based on chemical kinetics. **Explore** better catalysts for industrial processes based on current literature in chemical kinetics. **Design** a set of examples illustrating the differences between enantiomers, diastereomers, and meso compounds, a process utilizing zeolites for environmental remediation **Develop** a polarimeter experiment to measure the specific rotation of an unknown compound.

III SEMESTER PRACTICALS (CH3P25)

Semester	**III**
Paper code	**CH3P25**
Paper title	**Chemistry Practical III**
Number of Lab hours per week	**3**
Total number of Lab hours per semester	**33**
Number of credits	**2**

List of experiments

1. Determination of specific rotation by polarimetry
2. Kinetics- Saponification of esters
3. Salt Mixture Analysis-Instructions and Demonstration
4. Model salt Acid Radicals
5. Model salt Basic Radicals
6. Salt Mixture Analysis (5 sessions)
7. The heat of neutralization or enthalpy of dissolution of a salt or enthalpy of the interaction of chloroform and acetone (H-bond formation)
8. Repetition/viva-voce

Total 12 sessions

REFERENCES

1. Vogel's Qualitative Inorganic Analysis, by G. Svehla 7th Edition; Pearson (2012).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).
4. Athawale V. D. and Mathur P. Experimental Physical Chemistry, New Age International (2001).
5. An Advanced course in Practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2nd edition reprinted 2018.

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

LO1	Knowledge	**List** acid and basic radicals in different groups and the reagents used to identify them **Recall** the different tests to identify acids and basic radicals **Recall** the basic concepts of reaction kinetics **Recall** the different types of hydrolysis of esters **Recall** the concept of molecular chirality **Recall** the factors affecting optical rotation **Recall** the concept of enthalpy changes in chemical reactions
LO2	Understand	**Explain** ionic product, solubility product and relate these to the separation of cations in a given mixture and develop laboratory skill to classify the ions into the respective groups **Explain** the order and molecularity of saponification of esters **Represent** the rate law for saponification of esters **Relate** optical activity and molecular chirality **Explain** the principle of polarimeter **Classify** reactions into endothermic and exothermic based on enthalpy change
LO3	Apply	**Identify** the acid and basic radicals in a given salt and salt mixture **Predict** the order of a reaction based experimentally determined rate law
LO4	Analyse	**Analyze** the ions present in a given mixture qualitatively **Calculate** the rate constant based on experimental data **Calculate** the specific rotation of a given chiral compound **Calculate** the enthalpy change in utralization/dissolution/interaction of two solvents based on experimental data
LO5	Evaluate	**Apply** the principles of qualitative analysis to identify ions present in environmental/geological/industrial samples

		Interpret the reaction mechanism based on kinetic data **Determine** the concentration of unknown sample by measuring optical rotations of a series of working standards **Predict** the direction of heat flow based on experimental results
LO6	Create	**Predict** the feasibility of a reaction using enthalpy changes if entropy change and temperature are given

SEP Syllabus: B.Sc. Chemistry – 4th Semester

IV SEMESTER THEORY (CH425)

Semester	IV
Paper code	CH425
Paper title	Chemistry- IV
Total number of teaching hours per week	3
Total number of teaching hours per semester	45
Number of credits	3

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

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

SPECTROSCOPY- THEORETICAL CONCEPTS **13+2 hours**

Electromagnetic radiation- characteristics, frequency, wavelength, wave number and mathematical expressions connecting them. Types of Spectra: i) atomic and molecular ii) absorption and emission iii) continuous, band and line iv) rotational, vibrational (vibrational-rotational), electronic (UV & visible). Regions of the electromagnetic spectrum. Processes and spectral techniques associated with different regions. Born-Oppenheimer approximation.

Rotational spectra of diatomic molecules: Rigid rotor model. Derivation of the expression for rotational energy in terms of joule and cm^{-1}. Expression for rotational constant; selection rules, gross and quantum selection rules. Energy level diagram for a rigid rotor and rotational spectrum. Factors influencing rotational spacings.

Vibrational spectra of diatomic molecules: Frequency of oscillation of a simple harmonic oscillator. Hooke's law. Mathematical equation for fundamental vibrational frequency and fundamental wave number, significance of force constant, effect of reduced mass on vibrational frequency. Potential energy curve for a diatomic molecule behaving as a simple harmonic oscillator. Gross and quantum selection rules, energy level diagram. Expression for frequency of vibrational transition and zero-point energy. Fundamental vibrations, total degrees of freedom (translational, rotational, and vibrational), calculation of a number of fundamental vibrational frequencies for linear and non-linear molecules (e.g., H_2O, CO_2). Schematic representation of fundamental vibrations for H_2O, ***CO_2*** and discussion of their IR activity. Anharmonicity of vibrations of diatomic molecules, complexity of spectrum.

Raman spectra: Polarizability of molecules, elastic and inelastic collisions, Rayleigh and Raman scattering. Raman shift, Stokes and anti-Stokes lines. Selection rules (rotational Raman and vibrational Raman), intensity of Stokes and anti-Stokes lines, quantum theory of Raman effect, energy level diagram, rule of mutual exclusion. ***Differences between IR and Raman spectroscopy.*** Problem solving.

ALKYL HALIDES 8+ 2 hours

Nucleophilic substitution reactions: ***nucleophiles; leaving groups***; S_N2 reaction - kinetics, mechanism, free energy diagram and stereochemistry. S_N1 reaction - mechanism, free energy diagram and stereochemistry. ***Carbocations - structures and relative stabilities***. Factors affecting the rates of S_N1 and S_N2 reactions - structure of substrate (Hammond-Leffler postulate), concentration and strength of nucleophile, solvent (polar protic and polar aprotic), nature of leaving group. ***Substitution reactions in organic synthesis: functional group transformations using S_N2 reactions.***
Elimination reactions: E2 and E1 mechanisms; dehydrohalogenation - mechanism, bases used in dehydrohalogenation, comparison of S_N2 vs E2; comparison of S_N1 vs E1 in tertiary alkyl halides.

ALKENES AND ALKYNES 10+3 hours

Synthesis of alkenes *via* elimination reactions, Saytzeff's rule; exception to the rule when bulky base is used (mechanism and free energy diagram).
Acid-catalysed dehydration of alcohols with mechanism, ***dehydration of alcohols based***

on structure. Rearrangement of carbocations. Synthesis of alkynes by elimination of vicinal and geminal dihalides (mechanism excluded).

Hydrogenation of alkenes - syn and anti-addition. ***Hydrogenation of alkynes - syn and anti addition.***

Electrophilic addition of HX to alkenes - mechanism and free energy diagram, Markovnikov's rule, regioselectivity, peroxide effect. Stereochemistry of addition of HX to alkenes. Addition of water to alkenes: acid-catalysed hydration - mechanism, rearrangements. Oxymercuration-demercuration - regioselectivity. Hydroboration-oxidation -regiochemistry and stereochemistry. Electrophilic addition of bromine to alkenes – mechanism and stereospecificity.

Oxidative cleavage with hot basic potassium permanganate, cleavage with ozone (mechanistic details excluded). Electrophilic addition of chlorine to alkynes. Addition of HX to alkynes.

1,3-butadiene - electron delocalization; electrophilic attack on conjugated dienes, -1,4 addition; kinetic *vs* thermodynamic control; Diels-Alder reaction.

ALCOHOLS, ETHERS AND EPOXIDES 2+1 hours

Alcohols as acids; Conversion of alcohols into alkyl halides. Oxidation of alcohols. Synthesis of ethers by intermolecular dehydration of alcohols and Williamson ether synthesis (mechanism excluded); ***Cleavage of ethers (mechanism excluded).***

Synthesis of epoxides (mechanism excluded); Reactions of epoxides: acid and base catalysed ring opening of unsymmetrical epoxides, regioselectivity - examples (mechanistic details excluded).

ORGANOMETALLIC REAGENTS 3+1 hours

General characteristics, Classification based on the type of M-C bond; Examples. Preparations and reactions of Grignard reagents, organolithium compounds (synthesis of 1°, 2°, 3° alcohols, synthesis of alcohols from epoxides) and Gilman reagents (Reaction with halogenated compounds, epoxides and α, β-unsaturated carbonyl compounds). ***Comparison of reactivity and limitations.***

REFERENCES

1. Principles of Physical Chemistry, B. R. Puri; L. R. Sharma and M. S. Pathania, 48^{th} Edition, Vishal Publishing Co., 2021.
2. Introduction to Molecular Spectroscopy, C. N. Banwell and M. McCash, TMH Pub, 2010.
3. Physics of Atoms and Molecules, B. H. Bransden and Charles J. Joachain, 2^{nd} Edition, Pearson Education, 2017.
4. Organic Chemistry; G. Solomons, C. Fryhle, S. Snyder, 12^{th} Edition, Wiley, 2017.
5. Organic Chemistry; P. Bruice, 8^{th} Edition, Pearson Education India, 2020.
6. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, 2^{nd} Edition, Oxford University Press, 2014.
7. Organic Chemistry; Morrison and Boyd, 7^{th} Edition, Pearson Education India, 2011.
8. Organic Chemistry; B. Mehta and M. Mehta, 2^{nd} Edition, PHI Learning Private Limited, 2021.

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

LO1	Knowledge	**Recall** the regions of the electromagnetic spectrum where these spectra are observed; the assumptions of the rigid rotor model, the physical and chemical properties of these unsaturated hydrocarbons; the general formula and common examples of alkyl halides, the meaning of organometallic reagents. **Identify** common halogenating agents used in preparing alkyl halides, a nucleophile as a species that donates a pair of electrons to form a new bond, and the processes involved in synthesizing ethers and epoxides. **Identify and compare** the key factors influencing the reactivity of substrates in SN2 and SN1 reactions. **Recognize** a leaving group as the atom or group that departs during a substitution reaction.

		State the gross and quantum mechanical selection rules for rotational transitions, the Born-Oppenheimer approximation. **List** spectral techniques used in different regions of the electromagnetic spectrum, the characteristics of continuous, band, and line spectra, common examples and methods of preparation for alkenes, alkynes, and conjugated dienes, and the methods of converting alcohols into alkyl halides. **Define** atomic and molecular spectra and differentiate between them; alkenes, alkynes, and conjugated dienes, and recognize their general formulas and structures; alkyl halides and list their general properties and types (primary, secondary, tertiary); polar protic and polar aprotic solvents, nucleophiles, Raman shift. **Label** the different regions of the electromagnetic spectrum and their corresponding wavelength ranges.
LO2	Understand	**Explain** how different spectral processes (e.g., rotational, vibrational, electronic) correspond to specific regions, the significance of the force constant and its effect on vibrational frequency, the mechanism of nucleophilic substitution (SN1 and SN2) and elimination (E1 and E2) reactions involving alkyl halides, the transitions involved in rotational, vibrational, and electronic spectra, why specific transitions occur based on the selection rules, the concept of π-bonding in alkenes and alkynes and the delocalized π-system in conjugated dienes, the relative reactivity of organometallic reagents, the concept of intermolecular dehydration of alcohols for ether synthesis.

		Analyse the factors affecting the quality of a leaving group, such as bond strength and stability after departure. **Discuss** the role of reduced mass in determining the vibrational frequency of a diatomic molecule, how substrate structure, nucleophile strength, solvent type, and leaving group nature affect reaction pathways, the acid and base-catalyzed ring opening of epoxides, focusing on regioselectivity. **Derive** the expression for rotational energy in terms of units of energy (joules and cm^{-1}, a mathematical equation for the fundamental vibrational frequency and wavenumber of a diatomic molecule. **Describe** how different spectra are formed in terms of transitions, the role of alkyl halides as intermediates in the synthesis of other organic compounds, Markovnikov's and anti-Markovnikov's rules in the addition reactions of alkenes and alkynes, the Williamson ether synthesis and its applications. **Summarize** the factors affecting the reactivity of alkyl halides (e.g., steric effects, leaving group ability). **Illustrate** and interpret the potential energy curve of a diatomic molecule assuming harmonic oscillator behavior, and the stability trends of alkenes, alkynes, and conjugated dienes based on hyperconjugation and resonance.
LO3	Apply	**Apply** the Diels-Alder reaction to synthesize cyclic compounds using conjugated dienes, the Williamson ether synthesis to design the preparation of specific ethers.

		Analyse the factors affecting the quality of a leaving group, such as bond strength and stability after departure. **Classify** a given spectrum into continuous, band, or line categories, the degrees of freedom for linear and non-linear molecules. **Calculate** the rotational constant and energy levels for a given diatomic molecule, the number of fundamental vibrational frequencies for both linear and non-linear molecules. **Predict** the type of spectrum based on the energy transition data, the rotational spectrum of a diatomic molecule using the selection rule, the major products of addition, elimination, and oxidation reactions of alkenes and alkynes, the products of substitution and elimination reactions involving alkyl halides under given reaction conditions, the products of acid or base-catalyzed ring-opening reactions of unsymmetrical epoxides. **Solve** problems involving the preparation of alkenes and alkynes via elimination reactions. **Use** alkyl halides in synthetic pathways to create more complex organic molecules (e.g., alcohols, ethers, amines). **Demonstrate** the laboratory preparation of an alkyl halide from alcohols using halogenating agents. **Understand** how steric hindrance in the substrate affects SN2 reactions by hindering nucleophile attack; how SN2 reactions are used for functional group transformations in organic synthesis.

		Relate a given spectrum to its region of the electromagnetic spectrum. **Interpret** a rotational spectrum and correlate it with molecular properties; carbocation stability based on inductive effects, resonance, and hyperconjugation. **Sketch** the energy profile diagrams of SN1/SN/E1/E2 reactions.
LO4	Analyse	**Compare** the intensity of Stokes and anti-Stokes lines, the reactivity of organometallic compounds **Compare and contrast** SN1 and SN2 mechanisms based on factors like substrate structure, solvent effects, and nucleophile strength. **Differentiate** between substitution and elimination reactions based on reaction conditions and outcomes. **Analyse** the IR and Raman activity of fundamental vibrations for H_2O and CO_2, the role of carbocation stability in promoting SN1 reactions (primary, secondary, tertiary), the stereochemical implications of SN2 reactions on chiral alkyl halides, the regioselectivity in the acid or base-catalyzed ring-opening reactions of epoxides using examples. **Evaluate** which spectral technique is most appropriate for studying a given phenomenon. **Identify and explain** factors (e.g., molecular mass, bond length) affecting rotational spacings.

LO5	Evaluate	**Predict** whether a reaction will proceed via SN1/ SN2/ E1/E2 under specific conditions. **Predict and justify** the products and stereochemistry for substitution/elimination reactions. **Design** synthetic routes using alkyl halides as starting materials to prepare target compounds, incorporating multiple steps; synthetic routes to prepare complex organic compounds using alkenes, alkynes, or conjugated dienes as intermediates. **Propose** reaction conditions to favour either substitution or elimination reactions based on a given alkyl halide. **Combine** knowledge of reaction mechanisms to troubleshoot unexpected results in alkyl halide reactions. **Develop** strategies to selectively functionalize alkenes, alkynes, or conjugated dienes in multi-step syntheses. **Synthesize** polymers and advanced materials using conjugated dienes in polymerization reactions.
LO6	Create	**Design and solve** reaction mechanism problems by applying knowledge of SN1/SN2/E1/E2 reactions. **Evaluate** the environmental and safety implications of using alkyl halides in industrial and laboratory settings, the regioselectivity and stereoselectivity of reactions involving alkenes and alkynes. **Design** a synthetic pathway for a given ether or epoxide starting from alcohols or other precursors. **Critique** the efficiency of different methods for synthesizing alkyl halides from alcohols.

		Assess experimental data to determine the predominant reaction pathway (substitution vs. elimination) for a given alkyl halide reaction, how changes in molecular structure influence the rotational spectrum, the environmental impact and sustainability of industrial processes using alkenes and alkynes (e.g., ethylene and acetylene chemistry), the suitability of a method (e.g., dehydration vs. Williamson synthesis) for synthesizing ethers under given conditions.

IV SEMESTER PRACTICALS (CH4P25)

Semester	**IV**
Paper code	**CH4P25**
Paper title	**Chemistry Practical IV**
Number of Lab hours per week	**3**
Total number of Lab hours per semester	**33**
Number of credits	**2**

List of experiments

1. Qualitative tests for alkanes, alkenes, ethers and aromatic compounds
2. Oxidation of alcohol to aldehyde/ ketone
3. Qualitative tests for alcohol, aldehyde and ketone
4. Estimation of percentage of alcohol content by titrimetry
5. Preparation of aspirin and its characterization using UV-vis and IR spectra (2 sessions)
6. Estimation of aspirin by colorimetry
7. RBPT-4 sessions
8. Repetition/viva-voce

Total 12 sessions

REFERENCES

1. Vogel’s Textbook of Practical Organic Chemistry by B. S. Furniss, A. J. Hannaford, P. W. G. Smith, and A. R. Tatchell, 5th Edition, Pearson Education, 2015.
2. Vogel's Textbook of Quantitative Chemical Analysis by G. H. Jeffery, J. Bassett, J. Mendham, and R. C. Denney, 5th Edition, Longman Higher Education, 1994.
3. Manual of Methods of Analysis of Foods, Food Safety and Standards Authority of India (FSSAI), Government of India, 2015.

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

LO1	Remember	Relate the concepts of Beer-lambert's law to the colorimetric estimation of aspirin. Demonstrate by qualitative tests the chemical properties of functional groups. Recall the concept of molar calculations to get weight of organic compounds to be taken for reaction. List the reagents and equipment required for carrying out organic synthesis.
LO2	Understand	Compare the tests of aldehydes and ketones and illustrate by qualitative tests. Classify the given organic compound as saturated or unsaturated, aliphatic or aromatic by suitable tests. and draw inferences. Recognise the mechanism of reaction involved in organic synthesis.
LO3	Apply	Apply the concept of colorimetry to estimate organic compounds. Apply qualitative tests and identify the functional groups. Identify various reagents and suitable reaction conditions in the organic transformations.
LO4	Analyse	Draw inference from qualitative tests for functional groups. Analyse the practical yield of product formed.
LO5	Evaluate	Evaluate the calibration curve and estimate the amount of aspirin. Assess the feasibility of these methods/ reaction conditions in structurally related organic transformations.
LO6	Create	Design the suitable method for the synthesis of organic compound using appropriate precursor molecule.

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)

EVALUATION PATTERN - PRACTICALS

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