ST. JOSEPH'S UNIVERSITY

Bengaluru-27

Syllabus for

B.Sc. / B.Sc. (Honors) Chemistry

I –IV Semesters

2022-26

Department of Chemistry
School of Chemical Sciences
St. Joseph's University
Bengaluru- 560 027

Structure of the chemistry course for I- IV semesters of BSc (honors) 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 8 discipline core papers and 8 practical papers from I to VI semesters. For theory papers, internal Assessment (CIA) is given 40% weightage and End Semester Examination (SE) is given 60% the weightage. The practical internal assessment (PIA) is given 60% weightage and the end semester examination is given 40% weightage. CIA is based on written tests, seminars, assignments, quiz etc. End semester theory examination is for 2 h duration (60 marks) and practical examination is for 3 h 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	CH121 CH1P1	Chemistry I Practical I	56 44	**4** **4**	**40** **30**	**60** **20**	**100** **50**
II	CH221 CH2P1	Chemistry II Practical II	56 44	**4** **4**	**40** **30**	**60** **20**	**100** **50**
III	CH322 CH3P1	Chemistry III Practical III	56 44	**4** **4**	**40** **30**	**60** **20**	**100** **50**
IV	CH422 CH4P1	Chemistry IV Practical IV	56 44	**4** **4**	**40** **30**	**60** **20**	**100** **50**

Summary of credits for I-IV semesters

Semester	Code number	Title of the paper	No. of hours of teaching per week	Credit
I	CH121 CH1P1	Chemistry I Practical I	4 4	4 2
II	CH221 CH2P1	Chemistry II Practical II	4 4	4 2
III	CH322 CH3P1	Chemistry III Practical III	4 4	4 2
IV	CH422 CH4P1	Chemistry IV Practical IV	4 4	4 2

Name of the Degree Program	B.Sc. / B.Sc. (Honors) Chemistry
Discipline Core	Chemistry
Total Credits for the Program	186

Assessment: Weightage for assessments (in percentage)

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

B.Sc. / B.Sc. (Honors) Chemistry Semester I

Course Title: DSC-1: Chemistry-I	
Total Contact Hours: 56 h	Course Credits: 4
Formative Assessment Marks: 40	Summative Assessment Marks: 60
Duration of ESA/Exam: 2 h	

Course Pre-requisite(s):

PUC/12th standard or equivalent with Chemistry

Course Outcomes (COs):

At the end of the course, the student should be able to

- Explain basic laboratory practices like calibration of glassware, sampling, handling acids and safety precautions.
- Prepare the solutions after calculating the required quantity of salts in preparing the reagents/solutions and dilution of stock solution.
- Describe the limitations of classical mechanics which necessitated the development of quantum mechanics.
- Solve the Schrodinger's equation to obtain wave function for a basic type of potential in one dimension and predict the shapes of orbitals as well as probability distributions
- Justify the need for quantum mechanical structure of atoms
- Describe the periodicity in physical and chemical properties of elements in the periodic table.
- Explain the nature of bonding in organic compounds using concepts such as conjugation, resonance, etc.
- Explain methods of syntheses of alkanes, alkenes and alkynes along with their reactions.

B.Sc. Semester 1 – B.Sc. / B.Sc. (Honors) Chemistry

DSC-1: Chemistry-I

Semester	I
Paper Code	CH 121
Paper title	Chemistry-I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	52+4
Number of credits	4

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

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

ANALYTICAL CHEMISTRY –I **12+2 h**

Basic laboratory practices, calibration of glassware (pipette, burette and volumetric flask), sampling (solids and liquids), weighing, drying, dissolving, acid treatment. Guidelines for work in analytical laboratory and for performing quantitative determinations (volumetric and gravimetric).

Safety in chemical laboratory, prevention of fire and accidents, first aid. Precautions to be taken while handling toxic chemicals, concentrated/fuming acids and organic solvents. **(2 h)**

Language of analytical chemistry: Definitions of analysis, determination, measurement, techniques and methods. Significant figures, classification of analytical techniques. choice of an analytical method.

Errors and treatment of analytical data: Limitations of analytical methods; 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. (**6 h)**

Titrimetric analysis: Basic principle of titrimetric analysis. Classification, preparation and dilution of reagents/solutions. Equivalent masses of compounds, normality, molarity and mole fraction. Preparation of ppm level solutions, conversion factors. (**2 h)**

Acid -base titrimetry: Titration curves for strong acid vs. strong base, weak acid vs. strong base and weak base vs. strong acid titrations, selecting and standardizing a titrant. Quantitative applications. (**2 h)**

QUANTUM MECHANICS AND ATOMIC STRUCTURE 14 h

Limitations of classical mechanics - Black body radiation and photoelectric effect. de Broglie equation, Heisenberg's Uncertainty Principle and their significance.

Quantum Mechanics: Quantum mechanical operator- Hamiltonian operator, Normalized and orthogonal wave functions. Sign of wave functions. Postulates of quantum mechanics. Relation between Schrödinger's equation and standing wave, significance of ψ and ψ^2. Eigen values and functions. Particle in a one-dimensional box. Derivation for normalized wave function and energy. Particle in a 3-D box- equation for energy and wave function (no derivation). **(6h)**

Schrödinger's equation for hydrogen atom – qualitative description of results: Quantum numbers and their significance. Radial and angular wave functions for hydrogen atom. Radial distribution curves. Shapes of s, p and d orbitals. Probability diagrams. (**5 h)**

Multi-electron atoms: Pauli Exclusion Principle, Hund's rule of maximum multiplicity, the (n+l) rule, aufbau principle and its limitations- Electronic configurations of the elements (Z=1-30), effective nuclear charge, shielding/screening effect, Slater's rules. Variation of effective nuclear charge in periodic table. (**3 h)**

PERIODIC TABLE 14 h

The long form of periodic table, **s**, p, d and f-block elements. Detailed discussion of the following properties of the elements, with reference to s and p-block elements:

(a) Atomic radii (van der Waals) (b) Ionic and crystal radii. (c) Covalent radii

(d) Ionization enthalpy, successive ionization enthalpies and factors affecting ionization enthalpy. Applications of ionization enthalpy.

(e) Electron gain enthalpy; trends in electron gain enthalpy.

(f) Electronegativity, Pauling's electronegativity scale. Variation of electronegativity with bond order, partial charge, hybridization. Group electronegativity. (**8 h)**

Trends in the chemistry of the compounds of groups 13 to 17 (hydrides, carbides, oxides and halides). (**6 h)**

ORGANIC CHEMISTRY-I 12+2 h

Classification and nomenclature of organic compounds, hybridization, shapes of organic molecules, influence of hybridization on bond length and strength. **(2 h)**

Nature of bonding in Organic molecules

Formation of covalent bond, sigma and pi bonds, notations used to represent electron movements and directions of reactions-curly arrows, formal charges.

Localized and delocalized bonding, ***conjugation and cross conjugation with examples.***

Electronic displacements: Inductive effect, electromeric effect, resonance and hyperconjugation, Hückel's rule, aromatic, antiaromatic and nonaromatic species with examples. **(4 h)**

Strengths of organic acid and bases: Comparative study with emphasis on factors affecting pKa 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. Steric effect - relative stability of *trans* and *cis*-2-butenes.

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 explanation with examples. **(4 h)**

Chemistry of aliphatic hydrocarbons, **carbon - carbon sigma bonds**

Formation of alkanes: Wurtz reaction. Reactions of alkanes: free radical substitution, halogenation.

Carbon-carbon pi bonds: Formation of alkenes and alkynes by elimination reaction. Mechanism of E1, E2 reactions. Saytzeff and Hofmann eliminations. Addition of HBr to propene, free radical addition of HBr to propene. Addition of halogens to alkenes-carbocation and halonium ion mechanisms. Ozonolysis of alkenes, hydrogenation, hydration, hydroxylation and ***epoxidation of alkenes***, explanation with examples, addition of hydrogen halides to alkynes; conjugated dienes - 1,2 and 1,4- addition reactions in conjugated dienes. Diels-Alder reaction. (**4 h)**

Recommended Books/References:

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 9th edition, Saunders College Publishing, New York (2014).
2. Basic Inorganic Chemistry, F. A. Cotton, G Wilkinson and P. L. Gaus, 3rd Edition. Wiley. India 2007
3. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 2006.
4. Concise Inorganic Chemistry: J D Lee, 4th Edition, Wiley, (2021)

5. Organic Chemistry: Graham Solomons, Craig Fryhle, Scott Snyder, 11th Edition, Wiley (2014)
6. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education) 7th edition (2010)
7. Pine S. H. Organic Chemistry, Fifth Edition, McGraw Hill, (2007)
8. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., (2012), Oxford University Press.

Pedagogy: ICT tools, Chalk & Talk, Models & Charts.

Formative Assessment (Internal assessment) Theory	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation and class test	20
Seminars/Class work	10
Assignments/Discussions	10
Total	40

PRACTICALS (SEMESTER I)

Semester	I
Paper Code	CH1P1
Paper title	Practical-I
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	2

Course outcomes

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

- Calibrate common laboratory glassware like pipette, burette and volumetric flask.
- Conduct a variety of volumetric estimations such as acid-base and redox titrations.
- Purify/crystallize organic compounds by proper selection of suitable solvents.
- Synthesize different organic compounds using conventional/green methods.

PART- A Analytical Chemistry

Course objectives

- To prepare the standard/working solutions from source materials.
- To standardize the reagents and determination of analytes.

Course specific outcomes

- The students will be able to handle glassware, prepare and dilute solutions and perform the experiments with prepared reagents.
- The students will be able to determine the analyte through volumetric and gravimetric analysis and understand the chemistry involved in each method of analysis.
- The students will be able to deduce the conversion factor based on stoichiometry and in turn use this value for calculation.

LIST OF EXPERIMENTS

1. Calibration of pipette, burette and volumetric flask.
2. Estimation of Sodium hydroxide using potassium hydrogen phthalate.
3. Estimation of sodium carbonate and sodium bicarbonate in a mixture.
4. Estimation of alkali present in soaps/detergents.
5. Estimation of iron(II) using potassium dichromate/internal indicator.
6. Estimation of oxalic acid using potassium permanganate solution.
7. Standardization of silver nitrate and determination of chloride in a water sample.

PART- B Organic Chemistry

Course objectives

To get training on how to plan and execute single step synthesis of small organic molecules.

- To learn and get trained on how to purify a compound and to learn the crystallization techniques.
- To learn how to calculate percentage yield and to record physical constant.
- To understand the mechanism involved in the transformation.

Course specific outcomes

- Students gain the basic knowledge as how to select a solvent for crystallization of organic compounds and get trained as how to purify a compound.
- Students would understand the mechanism behind the reaction and role of catalysts in enhancing reaction rate and yield.
- Students would learn the importance of green methods over conventional methods.
- The students would be exposed to the safety measures to be taken to conduct reactions in the laboratory. and also learn how to manage by products and disposal of waste.

List of Experiments:

1. Methods of purification of organic compounds (Demonstration).
2. Preparation of acetanilide from aniline using Zn/acetic acid.
3. Synthesis of *p*-nitroacetanilide from acetanilide using nitrating mixture.
4. Bromination of acetanilide (i) conventional method and/or (ii) with ceric ammonium nitrate and potassium bromide (green method).
5. Bromination - preparation of tribromophenol from phenol.

Recommended Books/References

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis Sixth Edition, Pearson, 2009.
2. Practical Volumetric Analysis, Peter A C McPherson, Royal Society of Chemistry, Cambridge, UK (2015).
3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, 4th edition, Pearson Education (2009).
4. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry,

5th Ed., Pearson (2012).

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

Formative Assessment (Internal assessment) Practicals	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation	20
viva voce	10
Total	30

B.Sc. / B.Sc. (Honors) Chemistry Semester II

Course Title: DSC-2: Chemistry – II	
Total Contact Hours: 56 h	Course Credits: 4
Formative Assessment Marks: 40	Summative Assessment Marks: 60
Duration of ESA/Exam: 3 hrs	

Course Outcomes (COs)

At the end of the course the student should be able to:

- Explain the principles and concepts related to titrimetric analysis with reference to acid-base, precipitation and complexometric titrations.
- Handling of toxic chemicals, concentrated acids and organic solvents and practice safety procedures.
- Write the mechanisms of S_N1 and S_N2 reactions taking suitable examples.
- Illustrate types of aromatic electrophilic and nucleophilic substitution reactions with examples.
- Give a comprehensive description of the gaseous state in terms of molecular velocity, their distribution based on Maxwell-Boltzmann law, types of molecular velocities, molecular collision parameters, critical phenomena and liquefaction of gases.
- Explain important properties of liquid state such as viscosity, surface tension, refraction and parachor by defining them and elaborating on their experimental determination.
- Learn methods of determining molecular weights of solutes by measuring colligative properties and the concept of distribution law along with its applications.
- Describe the crystalline state in detail using the terms unit cell, Bravais lattices, Miller indices, Crystal systems, symmetry elements and lattice planes.

DSC-2: Chemistry – II

Semester	II
Paper Code	CH 221
Paper title	Chemistry-II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	52+4
Number of credits	4

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

ANALYTICAL CHEMISTRY II 14 h

Regression equation (least squares method), correlation coefficient (R^2), limit of detection (LOD), limit of quantification (LOQ), linear dynamic range (working range), sensitivity, selectivity, method validation, figures of merit of analytical methods**.** External standard calibration. **(4 h)**

Complexometric titration: Indicators for EDTA titrations - theory of metal ion indicators, titration methods employing EDTA - direct, back, displacement and indirect determinations. Application-determination of hardness of water. **(3 h)**

Precipitation titration: Titration curves, titrants and standards, indicators for precipitation titrations involving silver nitrate - Volhard's and Mohr's methods. (**2 h**)

Gravimetric Analysis: Requisites of precipitation, mechanism of precipitation, factors influencing precipitation, co-precipitation, post-precipitation. ***Advantages of organic reagents over inorganic reagents,*** reagents used in gravimetry - 8-hydroxy quinoline (oxine) and dimethylglyoxime (DMG). **(5 h)**

ORGANIC CHEMISTRY II 13+1 h

Nucleophilic substitution at saturated carbon: Mechanism of S_N1 and S_N2 reactions with suitable examples. Energy profile diagrams, stereochemistry and factors affecting S_N1 and S_N2 reactions. Basicity vs Nucleophilicity. (**4 h)**

Aromatic electrophilic substitution reactions: mechanisms, σ and π complexes, halogenation, nitration, sulphonation, ***Friedel - Crafts alkylation and acylation with their mechanism.*** Activating and deactivating groups. Orientation influence (Cl, $-NO_2$, CH_3, NH_2, OH). Ortho – para ratio. **(5 h**)

Aromatic nucleophilic substitution reaction: S_NAr mechanism, *ipso* substitution. Generation of benzyne with mechanism**.** **(5 h)**

STATES OF MATTER **25+3 h**

Gaseous state: ***Molecular velocity, collision frequency, collision diameter, collision cross section, collision number and mean free path.***

Maxwell-Boltzmann distribution of molecular velocities (most probable, average and root mean square velocities- mathematical derivation not required). Relation between RMS, average and most probable velocities and average kinetic energies (law of equipartition of energy).

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, vander Waals equation of state (No derivation) and application in explaining real gas behaviour. Critical phenomena - Andrews isotherms of CO_2, critical constants and their derivation from van der Waals equation, ***Experimental determination of critical constants.*** Continuity of states, Law of corresponding states. ***Joule-Thomson effect. Inversion temperature, application of J-T effect -*** liquefaction of air by Linde's process. **(8 h)**

Liquid state:

Surface tension: Definition ***and its determination using stalagmometer***, effect of temperature and solute on surface tension. **Viscosity**: Definition, coefficient of viscosity**.** ***Determination of viscosity of a liquid using Oswald viscometer.*** Effect of temperature, size, mass, shape of molecules and intermolecular forces on viscosity. **Refraction**: Specific and molar refraction- definition and advantages. Determination of refractive index by Abbes Refractometer. Additive and constitutive properties. **Parachor:** Definition, atomic and structure parachor, elucidation of structure of benzene and benzoquinone. Viscosity and molecular structure. Molar refraction and chemical constitution. (**6 h)**

Dilute solutions. Review of colligative properties. (Recall) Experimental determination of molar mass of solute by: (i) Beckmann method (ii) Landsberger method.

(**3 h**)

Distribution Law: Nernst distribution law - Statement. Distribution coefficient, factors affecting distribution coefficient, validity of distribution law, modification of distribution law when molecules undergo a) association b) dissociation. Application of distribution law in solvent extraction. Derivation for simple and multiple extractions. Distribution law in Parke's process of desilverisation of lead. (**4 h**)

Solid state:

Forms of solids**:** Anisotropy of crystals Unit cell and space lattice.

Laws of Crystallography: Law of constancy of interfacial angles, law of rational indices, law of symmetry (symmetry elements), crystal systems, Bravais lattice types and identification of lattice planes in cubic systems. Miller indices and its calculation, X–Ray diffraction by crystals: Bragg's law and derivation of Bragg's equation, single crystal and powder diffraction methods. Point defects in crystals. **(7 h**)

Recommended Text books/references:

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, Saunders College Publishing, New York (2014).
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry International 11th Ed., Oxford University Press (2018).
3. Physical Chemistry by Samuel Glasstone, ELBS (1982).
4. Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
5. Principles of Physical Chemistry, Puri, Sharma & Pathania, 47th edition. Vishal Publishing Co.2020
6. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). 7th edition (2010)
7. Physical Chemistry for the chemical and biological sciences – Raymond Chang: First Indian edition 2015.
8. Organic Chemistry: Graham Solomons, Craig Fryhle, Scott Snyder, 12th Edition, Wiley (2017).

Pedagogy: ICT tools, Chalk & Talk, Models & Charts

Formative Assessment (Internal assessment) Theory.	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation and class test	20
Seminars/Class work	10
Assignments/Discussions	10
Total	40

PRACTICALS - SEMESTER II

Semester	II
Paper Code	CH2P1
Paper title	Practical-II
Number of teaching hrs per week	4
Total number of teaching hrs per semester	44
Number of credits	2

Course Outcomes

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

- Estimate components in a mixture, nitrite in a water sample and hardness of water by volumetry.
- Estimate presence of nickel, barium and copper in solutions by gravimetry.
- Measure physical properties of a liquid such as density, viscosity and surface tension using specific instruments.
- Study the distribution phenomena of different systems and evaluate the corresponding distribution coefficient.

PART-A (Inorganic Chemistry)

Course Objectives

- To strengthen the concepts of mole and stoichiometry.
- To develop analytical skills of determination through titrimetry and gravimetry.

Course specific outcomes

The student will learn

- To prepare standard solutions.
- Techniques like precipitation, filtration, drying and ignition.
- Various titrimetric techniques and gravimetric methods.
- Calculation on the basis of mole concept and stoichiometry.

LIST OF EXPERIMENTS

a) TITRIMETRY

1. Estimation of carbonate and hydroxide present in a mixture.
2. Estimation of oxalic acid and sodium oxalate in a given mixture using standard $KMnO_4$/NaOH solution.

3. Standardization of potassium permanganate solution and estimation of nitrite in a water sample.
4. Standardization of EDTA solution and estimation of hardness of water.
5. Estimation of calcium in limestone.

b) GRAVIMETRY

1. Determination of Ba^{2+} as $BaSO_4$.
2. Estimation of Ni^{2+} as $Ni(DMG)_2$ complex.

PART -B (Physical Chemistry)

Course Objectives

- To learn various techniques for the measurement of viscosity, surface tension
- To study the effect of concentration on viscosity and surface tension.
- To understand the concept of distribution coefficient and Nernst Distribution law.

Course specific outcomes

The student will be able to

- Determine the density of liquids.
- Understand how viscosity and surface tension of liquids vary with concentrations.
- Explain the concept of distribution coefficient, and dissociation in a layer.

LIST OF EXPERIMENTS

1. Determination of density using specific gravity bottle and viscosity of liquids using Ostwald's viscometer (ethyl acetate, toluene, chlorobenzene or any other non-hazardous liquids).
2. Effect of concentration on the viscosity of a solution – sucrose solution.
3. Composition of binary mixture by viscosity method.
4. Determination of the density using specific gravity bottle and surface tension of liquids using Stalagmometer (ethyl acetate, toluene, chlorobenzene or any other non-hazardous liquids).
5. Determination of molar mass of non-electrolyte by Walker-Lumsden method.
6. Determination of partition/distribution coefficient - Acetic acid in water and butanol.

Recommended Books/References

1. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
2. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).
3. Athawale V. D. and Mathur P. Experimental Physical Chemistry, New Age International (2001).

Formative Assessment (Internal assessment) Practicals	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation	20
viva voce	10
Total	30

DSC-3: Chemistry-III

Semester	III
Paper code	CH 322
Paper title	Chemistry-III
Number of teaching hours per week	4
Total number of teaching hours per semester	52+4
Number of credits	4

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

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

CHEMICAL BONDING **19+1 h**

Ionic bonding: lattice energy, Born-Lande equation, Born-Haber cycle. Relation between lattice energy and melting point of an ionic solid.

Covalent bonding: octet rule and its limitations, Lewis structures of molecules and ions (when provided with sequence of atoms). Formal charge calculation for different atoms in molecules/ions. ***Partial covalent character of ionic bonds: Fajan's rules. Partial ionic character of covalent bonds. Calculation of % ionic character.***

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

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, sigma and pi bonds. Hybridisation: sp, sp^2, sp^3, sp^3d, sp^3d^2 with examples (inorganic molecules AB_n and AB_nL_m type with and without π-bonds).

Molecular orbital (MO) treatment of hydrogen molecule: linear combination atomic orbitals, bonding and antibonding orbitals, energy level diagram. MO energy level diagram of homonuclear diatomic molecules/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, electrical conductance of Li and Be.

ACIDS, BASES AND SOLVENTS **7+1 h**

Theories of acids and bases: ***Lowry-Bronsted concept***, conjugate acid-base pairs, amphiprotic substances, relative strengths of acid-base pairs, solvent system concept of acids and bases and 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. Applications of HSAB principle-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. Molten salts-classification with examples for each, and uses. 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). Solutions of alkali metals in liquid 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.*** Superacids and superbases: examples and Hammett acidity function (equation not required). Applications of superacids and superbases.

THERMODYNAMICS **18+1 h**

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 variables, 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.

Zeroth law- applications, thermodynamic temperature scale.

First law of thermodynamics-statement and mathematical form. Expression for work done in isothermal, adiabatic, isobaric, isochoric and cyclic processes. Work done in i) irreversible expansion and compression of an ideal gas, ii) reversible isothermal expansion and compression of an ideal gas (both isothermal and adiabatic conditions). Kirchoff's law (derivation). Limitations of first law, scope of second law, statements of second law of thermodynamics. Spontaneous and non-spontaneous processes, spontaneity and equilibrium. Driving force for spontaneous processes. Concept of entropy. Entropy changes in adiabatic and isothermal reversible expansions of an ideal gas. Change in 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 changes in phase transformations. Entropy changes in the system and surroundings for reversible expansion and irreversible processes; Carnot cycle- derivation of efficiency based on entropy concept. Entropy as a criterion for spontaneity. Physical significance of entropy and relation between entropy and probability.

Free energy–Gibb's free energy & Helmholtz free energy (work function), relation between w and ΔA and ΔG, standard free energy change of a reaction. Free energy criteria of spontaneity, Variation of G with T and P. Criteria of equilibria or spontaneity in terms of i) free energy ii) work function,

iii) enthalpy iv) internal energy v) entropy. Important thermodynamic relations using U=f(S,V), A=f(V,T), G=f(T,P)and H=f(P,S). The Maxwell equations and some applications of Maxwell's relations. Gibbs-Helmholtz equation–derivation; van't Hoff's reaction isotherm. Relation between free energy & equilibrium constant of a reaction.

Third law: Standard entropies, determination of absolute entropies of substances, residual entropy.

CHEMICAL KINETICS **6h**

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

Derivation of rate expressions for a second order reaction when a=b and a≠b. Methods of calculation of order of a reaction: i) integral 2and 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.

CATALYSIS **2+1 h**

Catalysis: general characteristics of catalytic reactions, catalytic poisons, catalytic promoters, positive and negative catalysts, auto catalysis, working of a catalyst. Types of catalysis– homogeneous and heterogeneous catalysis with examples, kinetics and mechanism of acid catalysed reactions, derivation of rate expression for general and specific acid catalysed reactions only. ***Theories of catalysis- intermediate complex theory, adsorption theory.***

REFERENCES

1. Principles of Physical Chemistry; B. R. Puri; L. R. Sharma and M. B. Pathania (47th edition); Vishal Chand Publishing Co.; (2016).
2. Principles of Inorganic Chemistry; B. R. Puri; L. R. Sharma and K. C. Kalia; (33rd edition) Vallabh Publications; (2016).
3. Text Book of Physical Chemistry; Samuel Glasstone; Macmillan India Ltd.
4. Physical Chemistry for the Chemical and Biological Sciences; Raymond Chang; (Indian Edition 2015); University Science Books.
5. Atkins Physical Chemistry; Peter Atkins and Julio de Paula; (Seventh Edition).; Oxford University Press; (2002).
6. Basic inorganic chemistry, F. A. Cotton, G. Wilkinson, Paul L. Gaus. 3rd ed., John Wiley India Pub (2009).
7. Inorganic chemistry, James H. Huheey, Ellen A. Keiter, Richard L. Keiter, 4th ed. Pearson education (2005).

8. Inorganic Chemistry, 7th edition, M. Weller, J. Rourke, T. Overton, F. Armstrong, Oxford Univ. Press. (1999).

Pedagogy: ICT tools, Chalk & Talk, Models & Charts.

Formative Assessment (Internal assessment) Theory	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation and class test	20
Seminars/Class work	10
Assignments/Discussions	10
Total	40

Course Outcomes	**Cognitive Level**	**At the end of the course, the student should be able to**
CO1	Knowledge	Recall definitions, laws, relationships in second and third law of thermodynamics, acids, bases and solvents, chemical bonding in molecules, ionic compounds, metals.
CO2	Understand	Explain concepts, relationships, theories, and models in acids, bases and solvents, molecular structure, chemical bonding, second and third law of thermodynamics.
CO3	Apply	Apply the bonding theories in predicting structure, bonding and magnetic properties of molecules, calculate efficiency of heat engines.
CO4	Analyze	Compare and contrast theories and generalisations of second and third law of thermodynamics, acids, bases and solvents, molecular structures, bonding.
CO5	Evaluate	Assess the applicability of theories of thermodynamics and kinetics, solvents, acids and bases, structure and bonding for a given system

Paper code: CH 322 Paper title: Chemistry- III

PRACTICALS - SEMESTER III

Semester	III
Paper code	CH3P1
Paper title	Practical-III
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	2

Course Outcomes

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

- Identify the acid and basic radicals in a given salt and salt mixture.
- 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.
- Analyze and distinguish the ions in a given mixture qualitatively.

PART-A (Inorganic Chemistry)

LIST OF EXPERIMENTS

1. Inorganic semi-micro qualitative analysis.
2. Inorganic semi-micro qualitative analysis.
3. Inorganic semi-micro qualitative analysis.
4. Inorganic semi-micro qualitative analysis.
5. Inorganic semi-micro qualitative analysis.
6. Inorganic semi-micro qualitative analysis.
7. Inorganic semi-micro qualitative analysis.

PART -B (Physical Chemistry)

Course outcomes

At the end of this course, students should be able to

- Understand the kinetics of chemical reactions.
- Determine the rate constant and order of chemical reactions from kinetic studies.

LIST OF EXPERIMENTS

1. To determine the rate constant and order of the reaction of the hydrolysis of an ester catalyzed by an acid.
2. To study the kinetics of saponification of ester and to determine its rate constant at room temperature.
3. To determine the order of reaction in iodine for the acid catalyzed iodination of acetone by colorimetric method.

Recommended Books/References

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

Formative Assessment (Internal assessment) Practicals	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation	20
Viva voce	10
Total	30

B.Sc. / B.Sc. (Honors) Chemistry Semester- IV

Course Title: DSC-4: Chemistry – IV	
Total Contact Hours: 56	Course Credits: 4
Formative Assessment marks: 40	Summative Assessment Marks: 60
Duration of ESA/Exam: 2 h	

DSC-4: Chemistry – IV

Semester	IV
Paper code	CH 422
Paper title	Chemistry-IV
Number of teaching hours per week	4
Total number of teaching hours per semester	52+4
Number of credits	4

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

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

SPECTROSCOPY- THEORETICAL CONCEPTS 12+2 h

Electromagnetic radiation- characteristics, frequency, wavelength and 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 electromagnetic spectrum. Processes and spectral techniques associated with different regions. Born Oppenheimer approximation.

Rotational spectra of diatomic molecules: Rigid rotor model. 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. 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) for linear and non-linear molecules. Calculation of 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, origin of P, Q and R branches (qualitative treatment only).

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 different types of spectra.

Problem solving.

SPECTROSCOPY - APPLICATIONS **14 h**

Electronic spectroscopy: Types of electronic transitions in organic molecules, meaning of λmax, Є and A, observed transitions in a typical UV-vis spectrum of simple organic molecules, effect of conjugation on λmax. Analytical uses of UV-vis spectroscopy.

Infrared (IR) spectroscopy: Modes of bending and stretching vibrations, functional group and fingerprint region, typical infra-red absorption frequencies of functional groups. Interpreting IR spectra, IR spectra of hydrocarbons and some functional groups containing heteroatoms; alcohols, ethers, difference in the IR spectra of 1^0, 2^0 and 3^0 amines, comparison of IR spectra of carboxylic acids, acid chlorides, esters and amide.

NMR spectroscopy: nuclear spin, origin of the signal, chemical shift, shielding and deshielding of protons, equivalent and non-equivalent protons. Integration of signal areas, signal splitting, spin-spin coupling, coupling constant. Interpretation of ^{1}H NMR spectra. Proton NMR and rate processes. Chemical exchange causing spin decoupling eg. ethanol.

Combined spectral problems using UV, IR and NMR techniques.

ALKANES AND CYCLOALKANES **9 +1 h**

Alkanes: Classification of types of hydrogen atoms. Physical properties of alkanes and cycloalkanes**.** Nomenclature of monocyclic cycloalkanes, cycloalkenes.

Sigma bonds and bond rotation, meaning of conformations, Newman projections, Sawhorse formula. Conformational analysis of ethane and butane. ^{1}H NMR spectra of bromoethane at room temperature and at low temperature.

Relative stabilities and ring strain of cyclopropane, cyclobutane and cyclopentane. Chair and boat conformations of cyclohexane and substituted cyclohexanes: axial and equatorial hydrogens. Conformations of methyl cyclohexane. ^{1}H NMR spectra of cyclohexane and undecadeuteriocyclohexane at ordinary temperature and low temperature.

Nomenclature of alkanes, 1,3- diaxial interactions of t-butyl group, end chapter problems

STEREOCHEMISTRY **11 + 1 h**

Constitutional isomers and stereoisomerism: constitutional isomers, enantiomers and diastereomers and chiral molecules. Chirality and stereochemistry. Molecules having one chirality 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 chirality centre, meso compounds, Fischer projection formulae. Separation of enantiomers: resolution, amines as resolving agents. Chiral molecules that do not possess chirality centre: diphenyls, allenes.

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

End chapter problems.

ALCOHOLS, ETHERS AND EPOXIDES **6 h**

(Recall, review: Nomenclature of alcohols, ethers and epoxides).

Alcohols as acids; conversion of alcohols into alkyl halides.

Synthesis of ethers by intermolecular dehydration of alcohols and Williamson ether synthesis, mechanism; cleavage of ethers (mechanism excluded).

Synthesis of epoxides (mechanism excluded); reactions of epoxides: acid and base catalysed ring opening of unsymmetrical epoxides, mechanism, regioselectivity – examples.

REFERENCES:

1. Principles of Physical Chemistry, B. R. Puri, L. R. Sharma, M. S. Pathania, (48th edition), Vishal publishing Co, (2019).
2. Fundamentals of molecular spectroscopy, C. N. Banwell, E. M. McCash, (4th edition), tata McGraw-Hill, (2008)
3. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan (5rd edition), Thomson Press, (2015).
4. Organic Spectroscopy, William Kemp, (3rd edition), Red Globe Press London, (2019).
5. Organic Chemistry, T. W. G. Solomons, C.B. Fryhle, Scott A. Snyder (12th Edition), Wiley India, (2016).
6. Organic Chemistry, R.T. Morrison and R.N. Boyd, (7th Edition), Prentice Hall, (2010).

Pedagogy: ICT tools, Chalk & Talk, Models & Charts.

Formative Assessment (Internal assessment) Theory	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation and class test	20
Seminars/Class work	10
Assignments/Discussions	10
Total	40

Course Outcomes	Cognitive Level	At the end of the course, the student should be able to
CO1	Remember	Recall various concepts of electromagnetic radiation, types of isomers; nomenclature of alkanes, cycloalkenes, alcohols, ethers and epoxides, stereochemistry.
CO2	Understand	Explain concepts, relationships, processes and models in spectroscopy, conformational analysis of alkanes and cycloalkanes, regioselectivity of ring opening in epoxides.
CO3	Apply	Predict molecular properties from spectral data, apply the concepts of spectroscopy to solve the spectral problems, apply the selection rules in identification of chirality and configuration.
CO4	Analyse	Compare and contrast various spectroscopic methods for their applications. Analyse the given spectral data and arrive at a probable structure. Analyse the given molecule for plane of symmetry, chirality and optical activity.
CO5	Evaluate	Assess the given conditions for ring opening of epoxides and evaluate regioselectivity. Based on the given spectral data evaluate the functional group/s present in the molecules.
CO6	Create	Design a suitable synthetic route for organic molecules and suggest a spectral method to assess the transformation.

PRACTICALS (SEMESTER IV)

Semester	IV
Paper Code	CH4P1
Paper title	Practical-IV
Number of teaching hours per week	4
Total number of teaching hours per semester	44
Number of credits	2

Course outcomes

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

- Apply the concept of analytical techniques like colorimetry for accurate chemical analysis.
- Synthesize small organic molecules using green and conventional methods.
- Characterize the synthesized organic compounds by UV-Vis/IR spectroscopy techniques.
- Apply the concept of spectroscopy to solve spectral problems.

Analytical and Organic Chemistry
LIST OF EXPERIMENTS

1. Colorimetric estimation of a dye.
2. Estimation of inorganic phosphate by Fiske-subbarow method.
3. Mechanochemical synthesis of Schiff base via solvent free method.
4. Preparation of azo dye by diazo coupling reaction.
5. Reduction of *m*-nitro phenol.
6. Oxidation of benzoin.
7. Recording of UV and IR for the prepared compounds and analysis of the spectral data-I.
8. Recording of UV and IR for the prepared compounds and analysis of the spectral data-II
9. Spectral problem solving 1: Structural analysis of compounds using NMR and IR spectral data.
10. Spectral problem solving II: Structural analysis of compounds using NMR and IR spectral data.
11. Repetition and VIVA.

Recommended Books/References

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis Sixth Edition, Pearson, 2009.
2. Practical Volumetric Analysis, Peter A C McPherson, Royal Society of Chemistry,

Cambridge, UK (2015).
3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry,4th edition, Pearson Education (2009).
4. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
5. An Advanced course in practical Chemistry, A. K. Nad, B. Mahapatra, A. Ghoshal, New Central Book Agency (P) Ltd, 2nd edition reprinted 2018.
6. Practical organic chemistry, A. K. Manna, Books and Allied (P) Ltd, 2018.

Formative Assessment (Internal assessment) Practicals	
Assessment Occasion/ type	**Weightage in Marks**
Continuous evaluation	20
Viva voce	10
Total	30

QUESTION PAPER PATTERN

END SEMESTER EXAMINATION (ESE)

St. Joseph's University, Bengaluru-27
B.Sc. End Semester Examination
(2022-23 onwards)
CHEMISTRY

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

Instructions

1. 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 25% portions from the mid semester exam portion and 75% weightage from the portion covered after mid semester examination.

MID-SEM EXAM PATTERN (MSE)

St. Joseph's University, Bengaluru-27
B.Sc. Mid Semester Examination
(2022-23 onwards)
CHEMISTRY

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

Instructions

1. 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 EIGHT 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**
Continuous evaluation	20
Viva voce	10
Total	**30**
End semester practical examination (ESPE)	**20**