

**VISVESVARAYA TECHNOLOGICAL UNIVERSITY
BELAGAVI**



Syllabus

M.Sc. in Chemistry

(Specialisation: Analytical Chemistry / Organic Chemistry)

(Effective from the Academic year 2024-25)

Programme Outcomes

1. **Advanced Knowledge and Understanding:** Graduates will have advanced knowledge of core areas in chemistry, including Analytical, Inorganic, Organic, and Physical Chemistry, along with emerging fields such as Biochemistry, Materials Chemistry, and Chemical Biology.
2. **Research Competency:** Students will be able to independently design, conduct, and analyze research, using both theoretical and practical approaches. They will be proficient in using modern scientific techniques and tools to solve complex chemical problems.
3. **Critical Thinking and Problem-Solving:** Graduates will develop strong critical thinking, analytical reasoning, and problem-solving skills, enabling them to address complex scientific and technical challenges.
4. **Ethics and Professionalism:** Students will understand and adhere to professional and ethical responsibilities in their research and professional activities, including the safe handling of chemicals and awareness of environmental and societal impacts.
5. **Communication Skills:** Graduates will be capable of effectively communicating scientific information, both in written and oral forms, to a variety of audiences, including scientists, non-specialists, and the general public.
6. **Interdisciplinary and Collaborative Skills:** Students will be prepared to work collaboratively in interdisciplinary teams, addressing broad scientific and societal challenges in areas like energy, health, and the environment.
7. **Lifelong Learning and Innovation:** Graduates will be committed to lifelong learning and staying current with advancements in chemistry and related fields. They will be prepared to innovate and adapt to new challenges in scientific research and industry.

I SEMESTER

FUNDAMENTAL CONCEPTS OF ANALYTICAL CHEMISTRY			
Course Code	MSC101	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:			
<ul style="list-style-type: none"> To familiarize statistical methods to validate analytical methods. To understand fundamentals and applications of separation techniques. To learn extraction and chromatographic methods for the separation and identification of different compounds. 			
Module-1			
<p>Analytical chemistry: Its functions and applications; analytical problems and procedures, analytical techniques and methods, method validation.</p> <p>Calibration and standards: Calibration, chemical standard and reference material.</p> <p>Quality in analytical laboratories: quality control, quality assurance and accreditation system.</p> <p>Errors in analytical measurements: measurement errors, absolute and relative errors, determinate and indeterminate errors and accumulated errors-sources, effects on results and control.</p> <p>Assessment of accuracy and precision: Accuracy and precision, standard deviation, relative standard deviation, pooled standard deviation, variance, overall precision, and confidence interval.</p> <p>Significance testing: Significance tests- Outlier, Q-test, F-test, t-test, and analysis of variance (ANOVA). Significant numbers.</p> <p>Calibration and linear regression: Calibration, linear regression, standard addition, internal standardisation, internal normalization, external standardisation.</p> <p>Figures of merit of Analytical methods: sensitivity and detection limit, linear dynamic range.</p> <p>Quality control and chemometrics: Control charts, collaborative testing and multivariate statistics.</p>			
Module-2			
<p>Principles of chromatography- Chromatographic separations and classification of principal chromatographic separations. Chromatographic mechanisms-sorption isotherms; adsorption systems-stationary and mobile phases, partition systems- stationary and mobile phases. Characterization of solutes-distribution ratio, retention factor, retention time and retardation factor.</p> <p>Sorption processes- adsorption, partition, ion- exchange and size exclusion. Chromatographic performance- Efficiency and resolution. Peak asymmetry- kinetic and temperature effects. Isolation of separated components.</p> <p>Quantitative and qualitative analyses.</p> <p>Thin layer chromatography (TLC) - Principles and procedures, stationary and mobile phases, solute-detection, alternative TLC procedures and applications of TLC.</p>			
Module-3			
<p>Gas chromatography (GC) - Principles and types. Mobile phases, Sample injections, columns and stationary phases. Temperature control and solute detection; thermal conductivity detector (TCD), flame ionization detector (FID), nitrogen-phosphorus detector (NPD) and electron capture detector (ECD). Instrument control and data processing. GC-procedures- temperature programming and special procedures used in GC. Quantitative and qualitative analyses.</p> <p>High Performance Liquid Chromatography (HPLC): Principles, mobile phases, solvent delivery systems, sample injection system, column and stationary phases. Solute detection -UV-visible,</p>			

fluorescence, refractive index and electrochemical detectors. Instrument control and data processing. Modes of HPLC. Optimisation of separations, qualitative and quantitative analyses.

Module-4

Ion-exchange chromatography (IEC): Principles, apparatus and instrumentation, and applications.

Size-exclusion chromatography (SEC): Principles, apparatus and instrumentation, and applications.

Affinity chromatography (AFC): Principles, methodology and applications. **Supercritical fluid chromatography (SFC):** Properties of supercritical fluids, instrumentation and operation variables, comparison of SFC with other chromatographic techniques, applications.

Supercritical fluid extraction (SFE): Advantages, instrumentation, choice of supercritical fluids, off-line and on-line extraction, applications.

Module-5

Electrophoresis (EP) and electrochromatography (EC): Principles- high performance capillary electrophoresis and capillary electrochromatography, running buffers, supporting medium, sample injection, solutes- detection, instrument control and data processing. Modes of EP and EC- capillary zone electrophoresis (CZE), micellar electrokinetic chromatography (MEKC), capillary gel electrophoresis (CGE), capillary isoelectric focusing (CIEF). Capillary electrochromatography (CEC), features, basis of separations. Qualitative analysis by CE and CEC and applications.

Solvent and solid phase extraction: Extraction techniques, extraction efficiency and selectivity. Solvent extraction (SE)-Extraction of organic acids and bases, extraction of metals. Methods of extraction and applications. Solvent phase sorbents, solid phase extraction (SPE) formats. Automated solid phase extraction. Solid phase micro extraction (SPME). Applications of SPE and SPME.

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001, John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prenticeHall, Inc. New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.

Course Outcomes:

CO1	Devise a scheme to be able to isolate organic acids, bases and neutrals through an extraction process.
CO2	Apply methods of distillation, sublimation, chromatography, filtration (including buchner filtration), evaporation, decantation, using magnetism, sieving and skimming to separate mixtures.
CO3	Understand the terms filtrate, residue, filtration, sediment, decant, distil, distillate, chromatogram and solvent front.
CO4	Know that mixtures are composed of constituents which are not combined.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X	X					
CO2	X	X					
CO3	X	X					
CO4	X	X	X			X	X

CONCEPTS OF INORGANIC AND BIOINORGANIC CHEMISTRY			
Course Code	MSC102	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:			
<ul style="list-style-type: none"> • To explore the structures of ionic crystals and simple molecules using the VSEPR model. • To understand acid-base concepts and chemical reactions in non-aqueous media, including ionic liquids and supercritical fluids. • To examine the chemistry of f-block elements. 			
Module-1			
<p>Chemical Periodicity: Review of periodic properties</p> <p>Structures and energetics of ionic crystals: Introduction, MX (NaCl, CsCl, ZnS) and MX₂ (fluorite, rutile, β-cristobalite, cadmium chloride and cadmium iodide) types. The perovskite and spinel structures. Thermodynamics of ionic crystal formation. Hydration energy and solubility of ionic compounds, Lattice energy, Born-Haber cycle, Born-Landé equation. The Kapustinskii's equation, Consequences of lattice enthalpies. Applications of lattice energetics. Ionic radii, factors affecting the ionic radii, radius ratio rules.</p> <p>Structures and energetics of inorganic molecules: Introduction, Bent's rule, Energetics of hybridization. VSEPR model for explaining structure of molecules including fluxional molecule. M.O. treatment of homo-nuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized π-bonding (CO_3^{2-}, NO_3^-, NO_2^-, CO_2 and N_3^-), M.O. correlation diagrams (Walsh) for triatomic molecules.</p>			
Module-2			
<p>Modern concept of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard-Soft Acids and Bases, Classification and Theoretical backgrounds. Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties) protic solvents (anhydrous H_2SO_4, HF and glacial acetic acid) aprotic solvents (liquid SO_2, BrF_3 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron. Super acids and super bases. Heterogeneous acid base reactions.</p> <p>Ionic liquids: Molten salt solvent systems, Ionic liquids at ambient temperature, Reactions in and applications of molten salt/ionic liquid media.</p> <p>Supercritical fluids: Properties of supercritical fluids and their uses as solvents. Supercritical fluids as media for inorganic chemistry</p>			
Module-3			
<p>Lanthanoid chemistry: General trends, Electronic, optical and magnetic properties. Abundance and extraction, General principles: conventional, solvent extraction and ion-exchange methods. Separation from monazite. Chemistry of principal oxidation states (II, III and IV). Stability of tetrahalides, dihalides and aqua ions of simple lanthanide compounds. Redox potentials. Uses: lanthanides as shift reagents, lanthanides as probes in biological systems. High temperature super conductors.</p> <p>Actinoid chemistry: General trends and electronic spectra. Occurrence and preparation of elements, Isolation of the elements: thorium and uranium, enrichment of uranium for nuclear fuel, uranium hydrides, oxides and chlorides. Chemical reactivity and trend. Chemistry of trans-uranium elements.</p> <p>Supramolecular Chemistry: Introduction, selectivity and Supramolecular Interactions.</p>			
Module-4			
<p>Structural and molecular biology: Introduction, The structural building blocks of proteins, the structural building block of nucleic acids. Metal ion interactions with nucleosides and nucleotides. General features</p>			

of DNA - metal complex interaction.

Bioenergetics: Introduction, Redox reactions in metabolism, the central role of ATP in metabolism. Kinetic stability of ATP, Mitochondrial flow of electrons from NADH to O₂. Phosphorylation and respiratory chain. Oxidative phosphorylation.

Vitamin B12 and Coenzymes: Structural feature, names of different forms, chemistry of cobalamin, biochemical functions of cobalamins, model compounds. Special characteristics of B12 co-enzyme. Photosystems.

Metal ion transport and storage: Iron storage and transport: Transferrin, ferritin, phosvitin and gastroferrin. Iron transport in microbes: siderophores, *in vivo* microbial transport of iron.

Oxygen transport and oxygen uptake proteins: Properties of dioxygen (O₂): thermodynamic and kinetic aspects of dioxygen as an oxidant, activation of dioxygen through complexation with metal ions. Haemoglobin (Hb) and Myoglobin (Mb) in oxygen transport mechanism: Introduction to porphyrin system, substituent effects on porphyrin rings, functions of Hb and Mb. Characteristics of O₂-binding interaction with Hb and Mb. Model compounds for oxygen carriers (Vaska's complex and cobalt(III) – Schiff base complexes). Hemerythrin and hemocyanin.

Electron transport proteins and redox enzymes: Iron – sulfur proteins (rubredoxins and ferredoxins) and cytochromes including cytochrome P450. Catalase and peroxidase: Structure and reactivity.

Superoxide dismutase: Structure and reactivity.

Module-5

Molybdenum containing enzymes: Aspects of molybdenum chemistry, Xanthine oxidase, aldehydes oxidase, sulfite oxidase, nitrogenase and nitrite reductase.

Non-redox metalloenzymes - Structure and reactivity: Carboxypeptidase-A, alcohol dehydrogenase, and carbonic anhydrase.

Medicinal Inorganic Chemistry: State of the Art, New Trends, and a Vision of the Future: Introduction, metals and human biochemistry, general requirements.

Disease due to metal deficiency and treatment: Iron, zinc, copper, sodium, potassium, magnesium, calcium and selenium.

Metal complexes as drugs and therapeutic agents: Introduction, Antibacterial agents, Antiviral agents, **Cancer Therapy:** Current Status and Mechanism of Action of Platinum-Based Anticancer Drugs. Non-platinum anticancer agents.

Gold-Based Therapeutic Agents: A New Perspective: Uses for the treatment of rheumatoid arthritis, **Metal-Based Radiopharmaceuticals:** Metal complexes as radio diagnostic agents.

ment of toxicity due to inorganics: General aspects of mechanism of metal ion toxicity, Mechanism of antidote complex with poison, rendering it inert: arsenic, lead, cyanide and carbon monoxide.

References

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
3. Inorganic Chemistry, 5th edition. G.L. Miessler, P. J. Fischer and D.A. Tarr, Pearson (2014).
4. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armstrong, Oxford University Press (2014).
5. Inorganic Chemistry, 4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
6. Introduction to Modern Inorganic Chemistry, K.M. Mackay and R.A. Mackay, Blackie Publication (1989).

7. Concepts and Models of Inorganic Chemistry 3rd edition. B.E. Douglas, D.H. McDaniel and Alexander, Wiley (2001).
8. Ionic liquids-Classes and Properties (Ed) by Scott T. Handy, Intech Publisher (2011).
9. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley and Sons Ltd., (2006).
10. Supramolecular Chemistry, Peter J. Cragg, Springer (2010).

Course Outcomes:

CO1	An understanding of the periodic properties of elements, the structures of ionic solids, and the calculations of their lattice energies.
CO2	Additionally, applying VSEPR concepts to analyze the structures of simple molecules.
CO3	Knowledge of various acid-base concepts and their applications across different fields, along with an understanding of the role of non-aqueous solvents in inorganic synthesis.
CO4	A comprehensive grasp of the chemistry of lanthanides and actinides, along with their practical applications.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X						
CO3	X	X	X				
CO4	X	X	X			X	X

STEREOCHEMISTRY AND ORGANIC REACTION MECHANISMS			
Course Code	MSC103	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:			
<ul style="list-style-type: none"> To understand detailed molecular structures of organic compounds. To learn bonding and chemical reactions of organic compounds. To study the different chemical reactions involved in organic synthesis. 			
Module-1			
<p>Stereoisomerism: Projection formulae [flywedge, Fischer, Newman and sawhorse], enantiomers, diastereoisomers, mesomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations.</p> <p>Optical isomerism: Conditions for optical isomerism: Elements of symmetry-plane of symmetry, centre of symmetry, alternating axis of symmetry (rotation-reflection symmetry). Optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.</p>			
Module-2			
<p>Geometrical isomerism: Due to C=C, C=N and N=N bonds, <i>E</i>, <i>Z</i> conventions, determination of configuration by physical and chemical methods. Geometrical isomerism in cyclic systems.</p> <p>Conformational analysis: Elementary account of conformational equilibria of ethane, butane and cyclohexane. Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanones and decalins.</p> <p>Conformational analysis of 1,2-, 1,3- and 1,4- disubstituted cyclohexane derivatives and <i>D</i>-Glucose, Effect of conformation on the course and rate of reactions.</p> <p>Stereoselectivity: Meaning and examples of stereospecific reactions, stereoselective reactions, diastereoselective reactions, regioselective, regiospecific reactions, enantioselective reactions and enantiospecific reactions.</p>			
Module-3			
<p>Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.</p> <p>Bonding in organic systems: Theories of bonding-molecular orbital approaches. Huckel molecular orbital theory and its application to simple π-systems: ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, cyclohexatrienyl, heptatrienyl, cycloheptatrienyl systems. Calculation of the total π-energy, and M.O. coefficients of the systems.</p> <p>Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, annulenes, heteroannulenes and polycyclic systems.</p> <p>Structure and reactivity: Brief discussion on effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.</p>			
Module-4			
<p>Methods of determining organic reaction mechanism: Thermodynamic and kinetic requirements for reactions, kinetic and thermodynamic control. Identification of products. Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Kinetic and stereochemical evidence, solvent effect. Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, arynes and ylides (Sulphur, nitrogen and phosphorous).</p>			

Aliphatic Nucleophilic Substitution reactions: Kinetics, mechanism and stereochemical factor affecting the rate of S_N^1 , S_N^2 , S_{RN}^1 , S_N^i , $S_N^{1'}$, $S_N^{2'}$, S_N^{1i} and S_{RN}^1 reactions, Neighbouring group participation.

Electrophilic substitution reactions: Kinetics, mechanism and stereochemical factor affecting the rate of S_E^1 & S_E^2

Module-5

Aromatic electrophilic substitution reactions: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier Haack reaction, Diazonium coupling, Gattermann-Koch reaction, Mercuration reaction.

Aromatic nucleophilic substitution reactions: S_N^1 , S_N^2 and benzyne mechanism, Bucherer reaction, von Richter reaction.

Mechanism of Addition reactions: Addition to C=C multiple bonds involving electrophiles, nucleophiles. Markownikoff's rule and anti-Markownikoff's rule.

Additions to carbonyl compounds: Addition of water, alcohol, bisulphate, HCN and amino compounds. Hydrolysis of esters.

Elimination reactions: Mechanism and stereochemistry of eliminations - E_1 , E_2 , E_{1cB} . *cis* elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution reactions, decarboxylation reactions. Chugaev reaction.

References

1. Stereochemistry of carbon compounds, Ernest L. Eliel.
2. Stereochemistry: P. S. Kalsi.
3. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
4. Organic Chemistry, Vol-I by I. L. Finar.
5. Advance Organic Chemistry, IV edition, Jerry March.
6. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechar J. Sundberg.
7. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
8. Reactive intermediates in Organic Chemistry, N. S. Isaacs.

Course Outcomes:

CO1	Optical and geometrical isomerism in organic compounds, with a focus on the application of stereochemistry in analyzing regioselective and regiospecific reactions.
CO2	Exploration of Hückel Molecular Orbital Theory (HMOT) and its applications to simple organic molecules
CO3	Understanding of aromaticity and techniques for determining reaction mechanisms.
CO4	Examination of nucleophilic, electrophilic, and elimination reactions.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X	X					
CO2	X	X					
CO3	X	X					
CO4	X	X	X			X	X

THERMODYNAMICS, KINETICS, PHOTO AND QUANTUM CHEMISTRY			
Course Code	MSC104	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:			
<ul style="list-style-type: none"> • To understand and study the rate of chemical reactions. • To familiarize the concept of photochemistry • To understand the concept of catalysis and enzyme kinetics • To know about free energy relationships 			
Module-1			
<p>Chemical Thermodynamics: Entropy: Physical significance, entropy changes in an ideal gas. Variation of entropy with temperature, pressure and volume. Entropy changes in reversible and irreversible processes.</p> <p>Free energy: Helmholtz and Gibbs free energies, Gibbs-Helmholtz equation and its applications, Maxwell's relations and its applications. Nernst heat theorem: its consequences and applications. Third law of thermodynamics: statements, applications and comparison with Nernst heat theorem.</p> <p>Partial molar properties: Physical significance, determination of partial molar volumes by intercept method and from density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs – Duhem equation. Derivation of Duhem-Margules equation.</p> <p>Fugacity: Relation between fugacity and pressure, variation of fugacity with temperature and pressure. Determination of fugacity of gases.</p> <p>Activity and activity coefficient: Variation of activity with temperature and pressure. Determination of activity co-efficient.</p> <p>Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions.</p>			
Module-2			
<p>Statistical thermodynamics: Objectives of statistical thermodynamics, concept of distribution, types of ensembles. Thermodynamic probability and most probable distribution law. Partition functions – definition, evaluation of translational, rotational and vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Sackur-Tetrode equation for entropy of translation function. Calculation of thermodynamic functions and equilibrium constants in terms of partition functions. Different distribution laws (Types of statistics): Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics (derivation of the three distribution laws). Comparison of Bose-Einstein and Fermi-Dirac Statistics with Maxwell-Boltzmann statistics. Problems and their solutions.</p> <p>Phase rule studies: Thermodynamic derivation of phase rule. Application of phase rule to the two component systems - compound formation with congruent melting point and incongruent melting points, Roozeboom's classification. Application of phase rule to three component systems- systems of three liquids and systems of two salts and water</p>			
Module-3			
<p>Chemical Kinetics: Complex reactions: Kinetics of parallel, consecutive and reversible reactions. Chain reactions: Branched chain reactions, general rate expression, Auto catalytic reactions (Hydrogen-Oxygen reaction), oscillatory reactions and explosion limits.</p> <p>Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates - derivation) and its applications to reactions in solution. Energy of activation, other activation parameters - determinations and their significance. Lindemann theory, Hinshelwood's theory of unimolecular reactions.</p>			

Reactions in solution: Ionic reactions - salt effects, effect of dielectric constant (single and double sphere models). Effect of pressure, volume and entropy change on the rates of reactions. Cage effect with an example.

Fast reactions- Introduction, study of fast reactions by continuous and stopped flow techniques, relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

Module-4

Photochemistry: Introduction to photochemistry, laws of photochemistry, laws of light absorption, quantum yield and its determination, factors affecting quantum yield, Actinometry - Uranyl oxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols for atoms and its significance.

Photochemical properties of electronically excited molecules, nature of changes on electronic excitation, shapes of absorption band and Frank Condon principle. Experimental techniques to determine the intermediates in photochemical reactions. Photosensitization: by mercury, dissociation of H₂. Photochemical kinetics of: Decomposition of CH₃CHO, formation of HI and HCl. Fluorescence and phosphorescence – theory and applications. Resonance fluorescence and quenching of fluorescence, Kinetics of collisional quenching (Stern-Volmer equation).

Module-5

Quantum Chemistry: Introduction to quantum mechanics: Schrödinger wave equation, time-independent and time dependent Schrödinger wave equation and the relation between their solutions. Eigen functions and Eigen values. Physical interpretation of wave function. Concept of operators – Laplacian, Hamiltonian, Linear and Hermitian operators. Angular momentum operators and their properties. Commutative and noncommutative operators. Normalization, orthogonality and orthonormality of wave functions. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for free particles, particle in a ring, particle in three dimensional box. Quantum mechanical degeneracy, tunnelling (no derivation). Wave equation for H-atom separation and solution of R, ϕ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. Eigen functions and Eigen values of angular momentum. Ladder operator method for angular momentum.

References

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone, 2nd Edn. Macmillan & Co Ltd., New York.
3. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
4. Chemical Kinetics by Frost and Pearson.
5. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.
6. Chemical Kinetics by L.K. Jain.
7. Photochemistry, Calvert and Pitts, Wiley, New York (1996).
8. Fundamentals of Photochemistry, Gohatgi-Mukherjee, New Age International Ltd., 1986.
9. Principles and Applications of Photochemistry, R. P. Wayne, Elsevier, New York (1970).
10. Photochemistry, Paul Suppan, RSC, London (1994).
11. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
12. Fundamentals of Chemical Kinetics, M. R. Wright, Harwood publishing, Chichesrer, 1999.
13. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.

Course Outcomes:

CO1

The completion of this course will enable the students to gain the knowledge on fundamentals and theoretical background on the concepts of chemical kinetics and theories

	of reaction rates
CO2	Students can able understand the basic principles of photochemistry, its experimental techniques and applications.
CO3	Applications of reaction kinetics which help in correlating the rates of biological and chemical reactions.
CO4	Apply the concept of free energy relations ships and kinetic isotope effect to understand reaction mechanisms

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X						
CO3	X	X				X	
CO4	X	X	X			X	X

INORGANIC CHEMISTRY PRACTICALS

Course Code	MSCL105	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	72	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives:

- To understand basic concepts by carrying out different experiments.
- To develop the skill for the qualitative and quantitative analysis of various samples.

PART – A

1. Determination of iron in haematite using cerium (IV) solution (0.02M) as the titrant, and gravimetric estimation of insoluble residue.
2. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.
3. Determination of manganese dioxide in pyrolusite using permanganate titration.
4. Quantitative analysis of copper-nickel in alloy/mixture:
 - i. Copper volumetrically using KIO_3 .
 - ii. Nickel gravimetrically using DMG
5. Determination of lead and tin in a mixture: Analysis of solder using EDTA titration.
6. Quantitative analysis of chloride and iodide in a mixture:
 - i. Iodide volumetrically using KIO_3
 - ii. Total halide gravimetrically
7. Gravimetric analysis of molybdenum with 8-hydroxyquinoline.
8. Quantitative analysis of copper(II) and iron(II) in a mixture:
 - i. Copper gravimetrically as CuSCN and
 - ii. Iron volumetrically using cerium(IV) solution
9. Spectrophotometric determinations of:
 - i. Titanium using hydrogen peroxide
 - ii. Chromium using diphenyl carbazide in industrial effluents
 - iii. Iron using thiocyanate/1,10-phenanthroline method in commercial samples
 - iv. Nickel using dimethylglyoxime in steel solution
10. Micro-titrimetric estimation of :
 - i. Iron using cerium(IV)
 - ii. Calcium and magnesium using EDTA
11. Quantitative estimation of copper (II), calcium (II) and chloride in a mixture.

PART – B

Semimicro qualitative analysis of inorganic mixtures containing **TWO** anions and **TWO** cations (excluding sodium, potassium and ammonium cations) and **ONE** of the following less common cations: W, Mo, Ce, Ti, Zr, V and Li.

References

1. Vogel's Text Book of Quantitative Chemical Analysis – 5th edition, J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition.
3. Spectrophotometric Determination of Elements by Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and Semimicro Inorganic Qualitative Analysis by A.I. Vogel.

6. Semimicro Qualitative Analysis by F.J. Welcher and R.B. Halin.
 7. 7. Quantitative Chemical Analysis by Daniel C. Harris, 7th edition, (2006).

Course Outcomes:

CO1	Determination of various analytes in different ore samples using volumetric, gravimetric, and spectrophotometric methods.
CO2	Exploration of the chemistry involved in redox, complexometric, and indirect methods.
CO3	Understanding the principles of semi-micro analysis in inorganic salt mixtures.
CO4	Ability to analyse the different inorganic salt mixtures.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X		X				
CO2	X						
CO3	X						
CO4	X	X	X				X

PHYSICAL CHEMISTRY PRACTICALS

Course Code	MSCL106	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	84	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives:

- To understand the rate of chemical reactions by carrying out kinetic experiments.
- To understand basic concepts of electrochemistry by carrying out several experiments

PART - A

1. Study of kinetics of hydrolysis of methyl acetate in presence of two different concentrations of HCl/H₂SO₄ and report the relative catalytic strength.
2. Study of kinetics of reaction between K₂S₂O₈ and KI, first order, determination of rate constants at two different temperatures and *E_a*.
3. To study the kinetics of saponification of ethyl acetate by conductivity method at two different concentrations of NaOH and report the relative catalytic strength.
4. Determination of partial molar volume of salt-water system (NaCl-H₂O/KCl-H₂O/KNO₃-H₂O) systems.
5. To study the kinetics of reaction between acetone and iodine - determination of order of reaction with respect to iodine and acetone.
6. Study the kinetics of decomposition of diacetone alcohol by NaOH, determine the catalytic coefficient of the reaction and comparison of strength of alkali.
7. Determination of energy of activation for the bromide-bromate reaction.
8. Kinetics of reaction between sodium formate and iodine and determination of energy of activation.
9. Determination of heat of solution of organic acid (benzoic acid/salicylic acid) by variable temperature method (graphical method).
10. Determination of degree of association of benzoic acid in benzene by distribution method.
11. To determine the eutectic point of a two component system (Naphthalene-*m*dinitrobenzene system).
12. Analysis of a binary mixture (Glycerol & Water) by measurement of refractive index.
13. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).

PART - B

1. Conductometric titration of a mixture of HCl and CH₃COOH against NaOH.
2. Conductometric titration of sodium sulphate against barium chloride.
3. pH titration of (a) HCl against NaOH (b) Copper sulphate against NaOH and (c) CH₃COOH/HCOOH against NaOH - determination of *K_a*.
4. Determination of equivalent conductance of weak electrolyte (CH₃COOH) at infinite dilution following Kohlrausch law.
5. Determination of dissociation constant and mean ionic activity coefficient of weak acids (CH₃COOH/HCOOH/ClCH₂COOH) by conductivity method.
6. Potentiometric titration of KI vs KMnO₄ solution.
7. Determination of dissociation constant of a weak acid (CH₃COOH/HCOOH/ClCH₂COOH) by potentiometric method.
8. Potentiometric titration of a mixture of halides (KCl+KI/KCl+KBr/KBr+KI) against AgNO₃.
9. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.

10. Potentiometric titration of $K_2Cr_2O_7$ against FAS determination of redox potential and concentration of Fe^{2+} ions.
11. Conductometric titration of oxalic acid against NaOH and NH_4OH .
12. Coulometric titration I_2 vs $Na_2S_2O_3$.
13. Determination of acidic and basic dissociation constant and isoelectric point of an amino acid by pH metric method.
14. Kinetics of photodegradation of indigocarmine (IC) using ZnO/TiO_2 as photocatalyst and study the effect of $[ZnO/TiO_2]$ and $[IC]$ on the rate of photodegradation.

References

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry – F. Daniels *et al.*
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico-Chemical Experiments – J. Rose.
7. Practical Physical Chemistry – S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry – D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry – R.C. Das and B. Behera, Tata Mc Graw Hill.

Course Outcomes:

CO1	After the completion of this course, the students can able to develop the experimental skill and theoretical interpretation of experimental results of many physical chemistry experiments of chemical kinetics in solution phase, thermodynamics, electrochemistry and spectrophotometry.
CO2	Students will be able to apply the learnings in academics, research and industries.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X	X	X				
CO2	X	X	X		X	X	X