Course No: MCHMCPC125
Title: Physical Chemistry (04 Credits))

Max. Marks: 100 | **Duration: 60 Contact hours**

Continuous Assessment: 28 marks | **End Term Exam: 72 Marks**

Course Objectives:

- To equip students with a comprehensive understanding of quantum mechanics foundations and solution of the Schrödinger equation;
- To learn solid-state characterization via X-ray diffraction, defect analysis, and theoretical models;
- To learn chemical dynamics including reaction rate theories, electron-transfer and chain reactions, and structure–reactivity correlations;
- To understand non-equilibrium thermodynamics encompassing entropy production, Onsager's relations, and solvent effects on electrolytes.

Course Learning Outcomes: After studying this course, the students will be able to

CLO1: understand the microscopic world and learn to solve the Schrodinger equation to evaluate energy of simple systems with or without potential energy.

CLO2: comprehend X-ray diffraction and its role in determining solid-state structure and electron density maps.

CLO3: know types of defects, their significance, and the evolution of solid-state theories from free electron approximation to finite potential field models.

CLO4: understand reaction rate theories, electron transfer mechanisms (Marcus theory and beyond), chain reaction types, and structure–reactivity relationships using LFER, Hammett, and related models.

CLO5: understand entropy production, Onsager's formalism, solvent effects on electrolytes, and far-from-equilibrium system behaviors.

Unit-I Quantum Chemistry-1 (15 Contact hours)

Quantum strangeness: Wave-particle duality of matter: outcomes of doublet slit experiment, Heisenberg's uncertainty principle and Copenhagen interpretation, Quantum mechanical paradoxes (Schrodinger's cat and Einstein's bubble thought experiments).

Schrodinger equation and operators: Time independent Schrodinger wave equations and its importance, physical interpretation of the wave function, Postulates of quantum mechanics. Introduction to operators. Algebra & commutation of operators with numerical problems. Linear and Hermitian operators, Hamiltonian operator. Eigen functions & eigen values. Orthogonality & normalization of wave functions.

Exactly solvable problems: Particle in a one/three-dimensional box. Tunneling effect. Harmonic oscillator & the rigid rotator problems. Solution of the Hydrogen-like atom problem, radial and angular wave functions.

Unit-II Structure and Theories of Solids (15 Contact hours)

Structure of solids: Lattice Planes and Miller indices; Bragg equation, Debye-Scherrer method of X-ray structural analysis of crystals, identification of cubic unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density.

Crystal defects and their types. Point defects: Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, Colour centres, Dislocations and their types.

Free electron theory of metals: The Drude and Lorentz Model, Sommerfield Model; Fermi-Dirac distribution function, Density of state and electronic heat capacity. Energy bands in general periodic potential-Kronig-Penney model. Qualitative band schemes for insulators, semiconductors and metals.

Unit-III Advanced Chemical Kinetics (15 Contact hours)

***Chemical Dynamics*:** Overview of reaction rate theories, Theories of Unimolecular reactions: Lindman, Hinshelwood, RRK and RRKM theories.
Electron transfer reactions: Rate laws for outer sphere electron exchanges, theories of Electron-Transfer Reactions; Classical Marcus Theory, solute driven and solvent driven processes, limitations of Marcus theory, ISM and Electron-transfer reactions, adiabatic and non-adiabatic self-exchange reactions, in transition metal complexes and organic molecules.
Structure Reactivity Relationships: Linear Free-Energy Relationships (LFER), Bronsted equation, Bell-Evans-Polanyi equation, Hammet and Taft relationships. Hammond postulates, the reactivity-selectivity principle.

Unit-IV Fundamentals of Irreversible Thermodynamics (15 Contact hours)

Basic principles of non-equilibrium thermodynamics: Second law of thermodynamics for open system, law of conservation of mass, charge and energy. Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity, Relation of uncompensated heat to other thermodynamic functions. Gibb's equation, entropy production, entropy production due to matter flow, heat flow, chemical reactions, charge flow; entropy production and efficiency of galvanic cells.
Concept of forces & fluxes, Onsager's theory of irreversible processes, phenomenological laws, their domain of validity. Principle of microscopic reversibility and Onsager relations, Chemical reactions near equilibrium. Curie–Prigogine principle. Electrokinetic phenomena and expressions for streaming potential, electro-osmotic pressure difference, streaming potential using the linear phenomenological equations. Dufour and Soret effects, Thermal Osmosis, Thermo mechanical effects, thermoelectric phenomena.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	2	3	3	2	2	3	3	2.6
CLO2	3	2	2	2	2	3	2	2.3
CLO3	3	3	2	2	2	3	3	2.6
CLO4	2	2	2	2	2	3	3	2.3
CLO5	2	3	2	2	2	2	3	2.3
Average PLO	2.4	2.6	2.2	2.0	2.0	2.8	2.8	2.4

Books Recommended:

1. Physical Chemistry; P. W. Atkins; Julio De Paula, Ed. 10th, Oxford University Press;2014.
2. Physical Chemistry- A Molecular Approach - D. A. McQuarie& J. D. Simon, University Science Books, 1997.
3. Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.
4. Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2014.

5. Quantum chemistry, Donald A. McQuarrie, Viva Books, 2016.
6. Quantum Chemistry, R.K. Prasad, 4th Revised Edition, New Age Publishers, 2020
7. Introduction to Solids, Azaroff, Tata McGraw,1993.
8. Solid State Chemistry and its Applications, West, Wiley, 2014.
9. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
10. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001.
11. Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003.
12. Solid State Chemistry An Introduction, 6th Edition, Elaine A. Moore, Jennifer Readman, CRC Press, 2025
13. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
14. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
15. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
16. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001.
17. An Introduction to Chemical Kinetics, Margaret Robson Wright, John Wiley & Sons, Ltd, 2004
18. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.
19. Thermodynamics of Irreversible Processes; DeGroot, Mazur; Dover;1986.
20. Introduction to Thermodynamics of Irreversible Processes; I. Prigogine; Wiley Interscience; 1967.
21. Thermodynamics for students of Chemsitry, Kuriacose, Rajaram, (S. Chand and Co., 1996).
22. Non-Equilibrium Thermodynamics, C. Kalidas, M. V. Sangaranarayanan, Macmillan India Limited, 2002
23. Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, USB, 1998.
24. Understanding non-equilibrium thermodynamics. G. Lebon, D. Jon, J. Casas Vasques. Springer, 2008.
25. Non-equilibrium thermodynamics, 2nd ed. Yasar Demirel. Elsevier, 2007.

Course No: MCHMCIC125
Title: Inorganic Chemistry (04 Credits)

Max. Marks: 100 | **Duration: 60 Contact hours**
Continuous Assessment: 28 marks | **End Term Exam: 72 Marks**

Course Objectives:

- To understand fundamental aspects of bonding in inorganic systems.
- To understand mechanism of complexation in multi-step reactions and factors affecting the mechanism and stability of the complexes.
- To compare crystal field and molecular orbital bonding theories vis-à-vis metal complexes.
- To understand π-acceptor ligand bonding characteristics and lanthanide coordination behavior/stability with diverse ligands.

Course Learning Outcomes: After studying this course, the students will be able to

CLO1: envisage and predict molecular geometry and comparative reactivity in diverse inorganic systems.
CLO2: utilize PSEPT and Styx conventions to rationalize bonding in main group compounds.
CLO3: correlate mechanisms of complexation process with their influencing parameters.
CLO4: obtain formation constants of complexes using different methods
CLO5: relate thermodynamic properties of complexes to their structural and electronic properties
CLO6: Correlate carbonyl IR spectra with structure; design lanthanide complexes for sensory/NMR/contrast applications.

Unit 1: Stereochemistry and bonding models in inorganic systems (15 Contact hours)

Bent's rule, isolobal analogy, polyhedral skeletal electron pair theory, and styx convention.
Bonding in main group compounds: types of bonds and topology of Boron clusters, selected examples of bonding in higher boranes; Carboranes and Metallacarboranes. Bonding in Boron–Nitrogen, Phosphorous–Nitrogen and Sulphur-Nitrogen compounds (Borazine, cyclophosphazenes, phosphonitrillic halides, sulphur Nitrides and polythiazyls).
Bonding in Metal pi acid Complexes and polymetallates: Coulson's treatment of bonding in case of metal carbonyls. Bonding in Dinitrogen and Dioxygen complexes. Bonding models of iso and hetereometallates.

Unit-II Metal-Ligand Equilibria in Solution (15 Contact hours)

Complexation process, Normal and abnormal trends in stepwise formation constants. Mechanisms of selected complexation processes. d^n configuration and lability, stability of uncommon oxidation states by complexation. Chelate effect, factors affecting stability of metal chelates. Ligand preorganization, Tertiary phosphine as ligand. Spectrophotometric Determination of composition and formation constants of complexes (Job's and Molar ratio method). Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn-Teller distortion and spectrochemical series.

Unit-III Bonding in Coordination Compounds and metal Clusters (15 Contact hours)

Experimental Evidence in favor of Metal Ligand Orbital Overlap; Adjusted crystal field theory. Molecular orbital theory of bonding in octahedral complexes: composition of ligand group orbitals; molecular orbitals and energy level diagram for sigma bonded ML_6; Effect of pi-bonding (Pi-donor and Acceptor Ligands). Molecular orbital and energy level diagram for bonding in Square-planar and Tetrahedral complexes. Factors favoring metal–metal bond, bonding in dinuclear metal clusters, cotton rationale and quadruple bonding, selected examples of bonding in dinuclear metal clusters. Characterization and bonding in Classical and non classical Hydrides (Kubas complexes).

Unit-IV Coordination Chemistry of pi acceptor ligands and Lanthanides (15 Contact hours)

Carbon monoxide as Pi acid ligand, Structure and bonding of mono- and poly-nuclear carbonyls (Coulson's treatment of bonding). Vibrational spectra of metal carbonyls for structural characterization. Structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes.

Comparison of d and f orbitals, Coordination numbers, stereochemistry and stability of lanthanide Complexes with nitrate, β-Diketonate, crown Ether and porphyrin type ligands. Homo and hetero dinuclear coordination compounds and coordination polymers of lanthanide ions. Utility of Lanthanide Complexes as Sensory Probes, NMR Shift Reagents and Contrast Agents.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	1	2	3	2	3	2.4
CLO2	3	2	2	2	2	3	3	2.4
CLO3	3	3	2	2	3	2	2	2.4
CLO4	2	3	2	2	3	3	2	2.4
CLO5	3	2	1	2	2	2	2	2.0
CLO6	2	2	2	2	1	3	3	2.1
Average PLO	2.7	2.5	1.7	2.0	2.3	2.5	2.5	2.3

Books recommended.

1. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.
2. Advanced Inorganic Chemistry; 5th. and 6th edn; F.A. Cotton, G. Wilkinson; Wiley;1998/1999.
3. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
4. Inorganic Chemistry; G. Wulfsberg; Viva; 2002.
5. Advanced Inorganic Chemistry; F.A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann; 6 th edn; John Wiley; 1999.
6. Chemistry of the Elements; 2nd edn; N. N. Greenwood, A. Earnshaw; Butterworth; 1997.
7. Inorganic Chemistry; 3rd edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.

8. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Saunders; 1977.
9. Chemistry of Elements; N. N. Greenwood & E. A. Earnshaw; 2 ndedn; Pergamon Press; 1997.
10. Coordination Chemistry; D. Banerjea; Tata McGraw Hill; 1993.
11. Lanthanide and Actinide Chemistry; Simon Cotton; 2nd Revised Edn.; John Wiley & Sons: West Sussex, England; 2006.
12. Inorganic Chemistry; Weller, Overton, Rourke, Armstrong; 6thEdn.; Oxford University Press; 2017 Reprint
13. Inorganic Chemistry; G. Wulfsberg; Viva Books Private Limited; 2005 Reprint
14. Chemistry of the Elements; 2ndEdn; N. N. Greenwood, A. Earnshaw; Elsevier; 2014 Reprint
15. Inorganic Chemistry; 3rdEdn; D. F. Shriver; P. W. Atkins; Oxford; 1999.

Course No: MCHMCOC125
Title: Organic Chemistry (04 Credits)

Max. Marks: 100 | **Duration: 60 Contact hours**
Continuous Assessment: 28 marks | **End Term Exam: 72 Marks**

Course Objectives:

- To impart a deep understanding of organic reaction mechanisms, and the experimental methods used to determine these.
- To explore the mechanistic aspects of nucleophilic substitutions in carbonyl compounds and their utility in organic synthesis.
- To develop advanced knowledge of stereochemistry, including the conformational analysis of complex organic molecules.
- To enhance the level of understanding of heterocyclic compounds and learn about their applications in materials and medicinal chemistry.

Course Learning Outcomes: After studying this course, the students will be able to

CLO1: apply mechanistic tools (e.g., isotopic labeling, KIE, stereochemistry, etc.) to determine organic reaction mechanisms.
CLO2: assess reactivity and synthetic utility of diastereoselective addition and nucleophilic acyl substitution in carbonyl compounds.
CLO3: analyze and predict stereochemistry of organic molecules with multiple chiral centers and conformationally constrained systems.
CLO4: demonstrate understanding of synthesis, reactivity, and applications of heterocyclic compounds in materials and pharmaceuticals.

Unit-I Reaction Mechanism and Chemical Reactivity (15 Contact hours)

Methods for studying reaction mechanisms: Types of reaction mechanisms. Transition states & Intermediates (Hammond postulate). Kinetic and thermodynamic evidence. Isotope labeling (^{13}C, ^{2}H, ^{18}O), primary and secondary Kinetic Isotope Effects (KIE). Structure of product, Influence of catalysts and solvents on reaction pathways. Detection of intermediates and stereochemical evidence.

Effect of structure on reactivity: Resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship. Substituent and reaction constants: significance and estimation, Taft equation.

Unit-II Chemistry of Carbonyl Functional Group (15 Contact hours)

Diasteroselectivity of Addition to Carbonyl Group in Acyclic and Cyclic Systems, Nucleophilic additions, stereochemical aspects through various models (Cram, Cram chelation and Felkin-Anh models, Cieplak model). Single enantiomers from diastereoselective Reactions.

Nucleophilic Substitution in Carbonyl Compounds

Mechanistic and synthetic aspects of nucleophilic substitution in carboxylic acids and their derivatives. Comparative reactivity of acid chlorides, anhydrides, esters, amides, and carboxylates.

Factors influencing reactivity and selectivity: Effect of substrates and leaving groups.

Reactions involving oxygen (H_2O, ROH, RCOO-, RCOOH), Nitrogen (aminolysis of acid chlorides and anhydrides) and carbon nucleophiles (conversion of esters to ketones using Grignard reagent). Hydrides as nucleophiles. Hydrolysis of amides and nitriles.

Unit-III Advanced Stereochemistry of Organic compounds (15 Contact hours)

Chirality in molecules with more than one chiral centre, Stereochemistry and configurations of alkylidine cycloalkanes, adamantanes, catenanes, bridged biphenyls, ansa compounds and cyclophanes. Racemic modification. Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.
Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanones, halocyclohexanones, Decalins, Aza decalins, decalols and decalones. Conformation of aldohexose sugars.
Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

Unit-IV Heterocyclic Compounds (15 Contact hours)

Hantzsch–Widman nomenclature of heterocycles, synthesis, structure and reactions of small heterocycles-oxirane, thirane, and azetidine, with emphasis on their applications as monomers in polymer synthesis. Chemistry of six-membered heterocycles- azines, and seven-membered rings including azepines, oxepines, and thiepines.
Heterocycles containing more than two heteroatoms: 1,3-Azoles, 1,2- Azoles oxadiazoles, and thiadiazoles. Heterocycles with ring-junction nitrogen: quinolizidine, indolizidine, and pyrrolo[1,2-a]pyrazine.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	2	3	3	3	1	2	**2.4**
CLO2	2	3	1	3	2	3	1	**2.1**
CLO3	2	3	1	3	2	3	1	**2.1**
CLO4	3	3	1	3	2	2	1	**2.1**
Average PLO	**2.5**	**2.8**	**1.5**	**3.0**	**2.3**	**2.3**	**1.3**	**2.2**

Books Recommended

1. Mechanism and Theory in Organic Chemistry – 3rd Ed., T.H. Lowry & K.S. Richardson, (Pearson) 1997.
2. Advanced Organic Chemistry 5th Ed., Part A & B, Francis A. Carey & Richard J. Sundberg, (Springer) 2008.
3. March's Advanced Organic Chemistry 6th Ed., Michael B. Smith & Jerry March, (Wiley) 2014.
4. Organic Chemistry 2nd Ed., Clayden, Greeves, Warren, and Wothers, (OUP) 2016.
5. Heterocyclic Chemistry – 5th Ed., J.A. Joule & K. Mills, (Wiley), 2010.
6. Heterocyclic Chemistry 3rd Ed., T.L. Gilchrist, (Pearson Education India) 2005.
7. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann, (George Thieme Verlag Stuttgart, New York) 1995.
8. Heterocyclic Chemistry, R. R. Gupta, M. Kumar, V. Gupta, (Springer) 2006.
9. Stereochemistry of Organic Compounds 7th Ed. - P.S. Kalsi. (New Age Inter.) 2012.
10. Stereochemistry of Organic Compounds – Ernest L. Eliel & Samuel H. Wilen, (TMH) 2007.

Course No: MCHMCMC125
Title: Mathematics for Chemists (02 Credits)

Max. Marks: 50 | **Duration: 30 Contact hours**
Continuous Assessment: 14 marks | **End Term Exam: 36 Marks**

Course Objectives:

- To introduce fundamental mathematical concepts relevant to chemical sciences and develop an understanding of their application in chemical investigations.
- To provide foundational knowledge of quantum mechanics, including its historical development and basic formulations for exploring microscopic phenomena.
- To familiarize students with numerical methods for solving complex mathematical problems such as systems of equations, integrals, differential equations, determinants, and eigenvalue problems.
- To equip students with practical skills in MS Excel as a tool for numerically solving mathematical problems encountered in chemical and scientific analysis.

Course Learning Outcomes:
After studying this course, the students will be able to

CLO1: learn basics of some mathematical concepts and their use in chemical investigations

CLO2: be able to understand the genesis of quantum mechanics and its basic formulations for understanding the microscopic world.

CLO3: appreciate the potential of numerical methods to solve the complex mathematical equations like simultaneous equations, integrals, differentials, determinants, eigen value problems etc.

CLO4: have in depth understanding of use of MS Excel as easily available tool to solve above

Unit-I Basic Mathematical Concepts for Chemists-I (15 Contact hours)

Functions and equations: Functions in chemical context, Representation of single variable functions; tabular and graphical. Special mathematical functions and their properties (Exponential, logarithmic and Trigonometric), Numerical calculations (Chemical) with logarithms. Equation of straight line, Linear plot and linear fit of the experimental data, Solving simultaneous linear equations; algebraic and graphical methods. (meaning and significance of slope and intercept with special examples from chemical equations), Solving polynomial equations in chemistry. Concept of linearization, linearizing non-linear equations.

Matrices and Determinants: The concept, addition and multiplication of matrices, evaluation of the value of determinants, properties of determinants, operations on matrices (The transpose of a matrix, The Complex Conjugate Matrix, The Complex Conjugate Transposed Matrix, The Trace of Square Matrix, The matrix of Cofactors), Matrices with Special properties (Symmetric, orthogonal, Singular, Hermitian, Unitary, Inverse Matrix) solving linear equations with matrices in chemistry.

Vectors: Geometric construction of vectors, vectors in two dimensions, Addition, subtraction and multiplication of vectors, matrix representation of vectors, Matrices for evaluation of vector multiplications. Matrix representation of Co-ordinate transformations following symmetry operations. Matrices and group theory.

Unit-II Basic Mathematical Concepts for Chemists-II (15 Contact hours)

Differentiation: The concept, rules and applications in chemistry (Finding maxima, minima and inflection points).
Integration: The concept, rules and applications in chemistry.
Differential Equations: Creation of differential equations using derivative of a function, Examples of differential equations in chemistry, First order and second order differential equations, their solution and examples in chemistry.
Statistics and Error Analysis: Systematic errors, Random Errors, Propagation of errors, Uncertainity in single variable, Combining Uncertainities in more than one variable;
Statistics of Repeated Measurements: The mean, variance and Standard deviation, sample variance and sample standard deviation, confidence intervals, Student t-Factors.
Linear Regression Analysis: The least square method, Finding the best Gradient and y-intercept, finding uncertainties associated with the gradient and y-intercept.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	3	1	2	3	3	**2.6**
CLO2	3	3	3	1	3	3	3	**2.7**
CLO3	3	3	3	1	2	3	3	**2.6**
CLO4	3	2	3	1	2	3	3	**2.4**
Average PLO	**3.0**	**2.8**	**3.0**	**1.0**	**2.3**	**3.0**	**3.0**	**2.6**

Books Recommended:

1. Maths for Chemists, Martin Cockett & Graham Dogget, 2nd Edition, RSC Publishing, 2012.
2. Maths for Chemistry, A Chemist's Toolkit of Calculations, Paul Monk & Lindsey J Munro, 3rd Edition, Oxford University Press, 2021.
3. Basic Mathematics for Chemists, P Tebbutt, 2nd Edition, 1998
   by (Author)
4. Maths for Chemistry: A chemist's toolkit of calculations, Paul Monk and Lindsey Munro 3rd Edition, Oxford University Press, 2021.
5. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
6. Physical Chemistry, A molecular Approach; Donald A. McQuarrie, John D. Simon.
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.

Course No: MCHMCGT125
Title: Group Theory and Applications (02 Credits)

Max. Marks: 50 **Duration: 30 Contact hours**
Continuous Assessment: 14 marks **End Term Exam: 36 Marks**

Course Objectives:

- To familiarize students about molecular symmetry, its significance and scope for chemical systems and processes.
- To familiarize students about the character table, its construction and significance.
- Understanding the mathematical context of spectroscopic methods.

Course Learning Outcomes: After studying this course, the students will be able to

CLO1: construct and interpret Character Tables.

CLO2: use of Character table to predict and interpret molecular properties.

CLO3: use character table as a tool to predict spectroscopic behavior of molecules.

Unit I. Group theory and Character tables (15 Contact hours)

Symmetry elements and assignment of point groups (Recapitulation). Combination and matrix representation of symmetry operations.
The Great Orthogonality Theorem: Elementary idea and consequences.
Reducible and Irreducible representations: Irreducible representations - Properties, proof and illustration of properties, Mullikan symbols. Character tables: Construction (C2V, C3V, C4V and D4 groups), structure of character table, linear and rotational functions (elementary idea), binomial and other polynomial functions (elementary idea). Reducible representations - Construction and reduction using the standard reduction formula.

Unit II. Applications of Group theory to Infra-red, and electronic spectroscopy (15 Contact hours)

Infra-red and Raman spectroscopy- Introduction, normal mode analysis- Cartesian coordinate method and internal coordinate method, symmetry of normal modes. Reducible representation of normal modes: Construction and reduction, selection rules, identification of IR and Raman active modes. Mutual exclusion principle.
Electronic spectroscopy: Introduction, transition dipole moment integral, selection rules. Electronic transitions between different states, polarization of electronic transitions.
Applications of symmetry to molecular chirality, polarity and hybridization.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	2	2	3	1	2	2	2	2.0
CLO2	2	2	3	1	3	1	3	2.1
CLO3	2	2	3	1	3	2	3	2.3
Average PLO	2.0	2.0	3.0	1.0	2.7	1.7	2.7	2.1

Books Recommended

1. Chemical Applications of Group Theory; 2nd edn.; F.A.Cotton; Wiley Eastern;(1994)
2. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.
3. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.
4. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E.Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc
5. Physical Methods for Chemists; R. S. Drago; 2nd edn; Saunders; 1992.

Course No: MCHMCLC125
Title: Laboratory Course in Chemistry-1 (04 Credits)

Max. Marks: 100 | **Duration: 120 Contact hours**
Continuous Assessment: 28 marks | **End Term Exam: 72 Marks**

Course Objectives:

- To develop conceptual and practical understanding of coordination compound synthesis, including design of synthetic procedures, stabilization of unusual oxidation states, and spectroscopic/thermal characterization techniques.
- To equip students with analytical proficiency in gravimetric, complexometric, and chromatographic techniques for separation and quantitative analysis of transition and main group metal ions.
- To train students in the identification of organic compounds through systematic observation of physical and chemical properties, including elemental and functional group analysis.
- To develop skills in separation, purification, derivatization, and quantitative estimation of organic compounds using standard laboratory techniques.
- To develop experimental skills for investigating reaction kinetics, viscosity, and thermochemical properties using various classical and instrumental methods.
- To enable students to analyze and interpret data from kinetic, viscometric, and calorimetric experiments to understand physical and chemical processes.

Course Learning Outcomes: After completing this laboratory course, students will be able to:

CLO1: synthesize and characterize coordination compounds of transition metals, applying concepts of redox behavior, in-situ stabilization, and spectroscopic and thermal analysis methods.

CLO2: perform gravimetric and complexometric estimations of binary metal ion mixtures and separate components using paper chromatography with appropriate mobile phases and chromatographic techniques.

CLO3: systematically identify organic compounds by analyzing their physical characteristics, elemental composition, and functional groups.

CLO4: separate, purify, and quantify organic substances from mixtures and apply derivatization and recrystallization techniques for characterization.

CLO5: perform kinetic experiments and evaluate reaction order, rate constants, and the influence of variables such as ionic strength.

CLO6: determine physicochemical properties such as viscosity and heat of neutralization, and apply viscometric data to estimate molecular parameters like solute radius and molecular mass of polymers.

SECTION A- INORGANIC CHEMISTRY

I. Synthesis and Characterization of the Coordination Compounds of Transition metals.

A. Theoretical appraise of first row Transition metal Coordination Chemistry.
B. Synthesis as a Laboratory Technique (Concepts, Calculations and Design of Synthetic procedures).
C. Selected preparations of the following coordination compounds with the specific objectives:

1 Tristhioureacopper(I)sulphate monohydrate:

i) Electron-neutrality Principle, ii) In-situ generation and Stabilization of unusual oxidation state, iii) Purification by recrystallization, iv) Observation of crystal morphology under microscope.

2 Trisethylenediaminecobalt(III) chloride:

i) Stabilization of Unusual Oxidation state, ii) Redox Chemistry of Co(II)/Co(III), iii) Resolution of racemic mixture.

II. Inorganic Quantitative Analyses.

A. ***Gravimetry:***
   i) Importance of weighing in Chemistry, Gravimetric Calculations
   ii) Precipitation process in homogenous mixtures, Precipitating agents, conditions of precipitation.
   iii) Precipitate processing (Digestion, Ignition); reducing precipitation errors (Co- and post precipitation)

B. ***Tritimetry:***
   i) Types and skill of titration, concept of Complexometric titrations, tritimeteric calculations. ii) Metallochromic Indicators: selection, structure, and mechanism of action. iii) Role and selection of buffers in Complexometreric titrations.

C. ***Separation and estimation of following Binary metal ion systems using Gravimetry &Tritimetry simultaneously:***
   i) Silver (Ag^{+}) as AgCl and Nickel (Ni^{2+}) as $[NiEDTA]^{2-}$ complex.
   ii) Nickel (Ni^{2+}) as Ni (DMG) complex and Magnesium (Mg^{2+}) as $[Mg\ EDTA]^{2-}$ complex.
   iii) Copper (Cu^{2+}) as CuSCN and Magnesium (Mg^{2+}) as $[MgEDTA]^{2-}$ complex.

III. Paper Chromatography

(i) Methods of paper chromatography (Ascending, Descending and Radial)
(ii) Comparative mobile phase study of separating binary and ternary metal ion mixtures. Chromatogram analysis and Interpretation.

SECTION B-ORGANIC CHEMISTRY

1. Qualitative Analyses of Organic Compounds

(I) Physical Properties: Physical state, colour, odour, solubility behaviour and melting / boiling points.

(ii) Chemical Properties
- **(a) Flame test**
- **(b) Detection of elements:** Nitrogen, Sulphur and Halogens
- **(c) Detection of Functional Groups:** Detection of Carbohydrates, unsaturation, carboxylic acids, carbonyl compounds, phenols, alcohols, halides, amines, amides, imides, ureas, thioureas, nitro compounds and hydrocarbons.

2. Separation, Purification and identification of Organic compounds from a two-component mixture: Derivatization and recrystallization.

3. Quantitative Estimation of the following compounds

(a) Glucose.

(b) Glycine

SECTION C-PHYSICAL CHEMISTRY

A. Chemical Kinetics

1. Determination of order of reaction between $K_2S_2O_8$ and KI by Initial rates method using clock reaction.
2. Compare the effect of ionic strength on the rate constant of persulphate-iodide reaction and iodide-Fe(III) reactions using clock method.
3. Determination of the rate constant of inversion of cane sugar catalysed be HCl using polarimeter.

B. Viscometery

1. Investigation of variation of viscosity with conc. and determination of unknown concentration and the radius of solute molecule by viscosity measurement.
2. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method.

C. Calorimetry

1. Determination of heat of neutralization of a strong acid with a strong base.
2. Determination of heat of neutralization of a weak acid with a strong base.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	3	3	3	3	3	3.0
CLO2	3	3	2	3	3	2	3	2.7
CLO3	3	3	3	2	3	3	3	2.9
CLO4	3	3	3	2	3	3	3	2.9
CLO5	3	3	2	3	2	3	2	2.6
CLO6	3	3	2	3	3	2	3	2.7
Average PLO	3.0	3.0	2.5	2.7	2.8	2.7	2.8	2.8

Books Recommended:

1. Vogel's Textbook of Quantitative chemical Analysis; 5^{th}edn; Jeffery, Bassett; (ELBS, 1989).
2. Quantitative Analysis; 6^{th}edn; Day, Underwood (Printice Hall, 1993).
3. Analytical Chemistry, 6^{th}Ed; D. Christian, Wiley.
4. Quantitative Analysis; 6^{th}edn; Day, Underwood (Printice Hall, 1993).
5. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, **1992.**)
6. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., **1989).**
7. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, **1999)**.
8. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, **1996)**
9. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-**2000).**
10. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
11. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
12. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.