Course No: MCHMCPC225
Title: Physical Chemistry (04 Credits)

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

Course Objectives:

- To understand the fundamental principles of quantum chemistry, including angular momentum theory, approximation methods, and perturbation theory, and apply these to atomic systems.
- To explore the electrical, dielectric, and magnetic properties of solids, including semiconductors, superconductors, and magnetic materials, and understand their technological applications.
- To study the synthesis, characterization, and applications of functional soft materials, such as hydrogels, Langmuir-Blodgett films, and liquid crystals.
- To analyze ion-solvent and ion-ion interactions in electrolyte solutions and understand theories governing their conductance and activity.
- To inculcate critical thinking and problem-solving skills through the application of physical chemistry concepts to real-world materials and systems.

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

CLO1: explain and apply quantum mechanical concepts like angular momentum, spin-orbit coupling, variation, and perturbation methods to simple atomic and molecular systems.
CLO2: analyze the behavior and properties of semiconductors, dielectrics, superconductors, and magnetic materials, and explain their operational principles and technological relevance.
CLO3: describe the synthesis, classification, and applications of soft materials, such as hydrogels, Langmuir-Blodgett films, and liquid crystals, including their physicochemical behavior.
CLO4: interpret ion-ion and ion-solvent interactions using models like Debye-Hückel and Bjerrum's theory and evaluate the conductance behavior of electrolyte solutions.
CLO5: design and evaluate materials or processes involving physical chemistry principles for applications in electronics, sensors, biomedicine, and materials science.
CLO6: understand entropy production, Onsager's formalism, solvent effects on electrolytes, and far-from-equilibrium system behaviors.

Unit-I Quantum Chemistry-2 (15 Contact hours)

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, Atomic term symbols, term separation of pn and dn configurations, spin- orbit coupling, Zeeman splitting.
Approximation methods: Variation method: the Variation theorem, linear variation principle, application to hydrogen atom and helium atom. Perturbation method: first order (non-degenerate & degenerate). Application of perturbation method to helium atom and anharmonic oscillator.

Unit-II Electric, dielectric and magnetic properties of Solids (15 Contact hours)

Semiconducting Properties: Intrinsic & extrinsic semiconductor (n-type & p-type), temperature dependence of charge carriers, p-n junction- devices based on p-n junction (tunnel diode, injection laser).

Superconducting properties: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, absorption of em radiations and Josephson effect. BCS theory of superconductivity, applications of superconductors.
Dielectric Properties: Dielectric constant, Polarization and Polarizability, Piezoelectricity, pyroelectricity and ferroelectricity, applications of dielectric materials.
Magnetic properties: Origin of magnetism in solids, diamagnetism, paramagnetism (Langevin's and quantum mechanical formulations), ferromagnetism (Wiess theory), antiferromagnetism and ferrimagnetism. Temperature dependence of magnetization.

Unit-III Hydrogels, Langmuir Blodgett Films and Liquid crystals (15 Contact hours)

Hydrogels: Introduction, Classification of hydrogels based on type of source, crosslinking and composition. Introduction to stimuli responsive hydrogels and their types. Rheological properties of hydrogels (steady-state, oscillatory and thixotropic behavior). Characterization of hydrogels. Applications of Hydrogels in adsorption, 3D printing, shape memory materials, drug release and other biomedical applications.
Langmuir-Blodgett Films: Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.

Liquid Crystals: Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications – Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals

Unit-IV Electrochemistry-1 (15 Contact hours)

Ion solvent Interactions: Non structural (Born) treatment and an introduction to structural (Ion-dipole, Ion-quadruple) treatments of ion-solvent interactions.
Ion-Ion Interactions: Activity and activity co-efficient. Debye-Huckel theory of activity coefficients of electrolyte solutions; derivation of Debye-Huckel limiting law, validity and extension to high concentrations; ion-pair formation-Bjerrum model.
Conductance of electrolyte solutions: Mobility of ions, mobility and conductivity, Einstein relations, dependence of molar conductance on concentration, Theories of Conductance: Debye-Huckel-Onsager conductance equation, Empirical extensions to the Debye-Huckel-Onsager Equation, Fuoss-Onsager equation.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	3	1	3	3	3	2.7
CLO2	3	2	2	2	2	3	2	2.3
CLO3	3	3	2	1	3	3	3	2.6
CLO4	2	2	2	1	3	3	3	2.3
CLO5	2	2	2	2	2	3	3	2.3
CLO6	3	3	2	2	3	2	3	2.6
Average PLO	2.7	2.5	2.2	1.5	2.7	2.8	2.8	2.5

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, ELBS , Oxford, 2009.
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, 2009.
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. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
13. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola,New York, 2001.
14. Properties of Liquids and Solutions; J.N. Murell and E. H. Boucher; John Wiley & Sons Ltd; 1982.
15. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
16. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
17. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
18. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
19. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
20. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
21. Molecular Thermodynamics of Electrolyte Solutions, Lioyd L Lee, World Scientific, 2008.
22. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.
23. Modern Electrochemistry Volume 1, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.

Course No: MCHMCIC225
Title: Inorganic Chemistry-Reaction mechanism (04 Credits)

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

Course Objectives:

- Understanding of reaction rates and their dependence on various extrinsic and intrinsic factors.
- Understanding of optimized reaction conditions, including nature of reagents and catalysts for optimum product formation.
- Understanding the factors promoting inner and outer sphere electron transfer reactions between coordination complexes and differentiation between two types of reactions.
- Significance, reactivity patterns and comparative stabilities of the different classes of OMC.
- Analyze decomposition pathways, catalytic cycles, and bioorganometallic mechanisms in organometallic reaction systems.

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

CLO1: predict of reaction rates, mechanism of reactions and nature of products.
CLO2: select the catalyst and optimum reaction conditions for better yields.
CLO3: design desired coordination compounds for useful applications.
CLO4: to differentiate between inner and outer sphere electron transfer reactions based on nature of reactants and reaction rates.
CLO5: evaluate industrial catalytic processes (hydrogenation, hydroformylation) using TON/TOF metrics and mechanistic principles.

Unit I: Ligand Substitution Reactions in Square-Planar complexes (15 Contact hours)

Energy profile of reactions, reaction intermediates and transition states.
Types of substitution reactions. Mechanistic classification of substitution reactions - Dissociative, Associative, and Interchange mechanism. Empirical criteria to differentiate the mechanism of substitution reaction. Rate laws.
General reaction mechanism of square planar complexes, K_S and K_Y pathways (S=solvent, Y=nucleophile). Factors effecting reaction rates: Nature of entering group - nucleophilicity and basicity, nucleophilic constants npt and npt° scales. Trans-effect - Theories and application in synthesis. Trans influence. Cis-effect. Leaving group. Central metal ion.

Unit II: Ligand Substitution Reactions in Octahedral Complexes (15 Contact hours)

Kinetic and thermodynamic stability. Identification of inert and labile complexes.
Substitution in octahedral complexes: Replacement of coordinated water- Eigen-Wilkins mechanism. Classification of metal ions based on water exchange rates. LFAE considerations. Anation reactions.
Base hydrolysis: Mechanistic details. Conjugate base (CB) mechanism, Rate of base hydrolysis. Case studies of base hydrolysis - effect of base concentration, nucleophiles, ligands with acidic protons and reactant isomerism.

Acid hydrolysis: Mechanism, case studies of complexes without π-donor/acceptor ligands, with π acceptor ligands and iii) with π-donor ligands.
Substitution reactions without breaking of metal-ligand bond.

Unit III: Electron transfer Reactions (15 Contact hours)

Classification of oxidation-reduction reactions. Inner sphere electron transfer reaction (ISETR) mechanism - Taube reaction, elementary steps, precursor and successor complexes. Requirements for ISETR. Bridging ligand effects, case of multidentate ligands, electron transfer through extended bridges, double bridged intermediates.
Outer sphere electron transfer reaction mechanism - Elementary steps, precursor and successor complexes. Chemical activation - Frank-Condon, ΔM-L (metal-ligand bond distance), electronic configuration, orbital symmetry considerations.
Elementary idea to Marcus equation - Marcus cross equation.
Differentiation of inner sphere and outer sphere electron transfer reactions.

Unit IV Reaction mechanism in organometallic systems (15 hours)

Stability of organometallic compounds, Mechanisms of thermal instability (Decomposition pathways), oxidation and hydrolysis. Mechanisms of Cyclometallation, intramolecular alkane elimination and Beta hydrogen transfer, reactions. Comparative thermal stabilities of different classes of sigma organometallic compounds. Tolman catalytic loop, Catalytic efficiency: TOF, TON and e.e. Mechanistic investigations of selected industrial catalytic processes: Hydrogenation, Hydroformylation, and Monsanto Acetic acid reaction. Bioorganometallics (Ru(II) anticancer compounds, vitamin B_{12})

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	3	2	3	3	2	2.7
CLO2	3	3	2	2	3	3	2	2.6
CLO3	3	3	3	3	3	3	2	2.9
CLO4	2	3	3	3	2	3	2	2.6
CLO5	2	2	2	2	2	3	2	2.1
Average PLO	2.6	2.8	2.6	2.4	2.6	3.0	2.0	2.6

Books Recommended

1. Advanced Inorganic Chemistry, 6th ed. /5th ed. F.A. Cotton , G. Wilkinson (Wiley 1999/1988)
2. Inorganic Chemistry, 4th ed. J. E. Huheey, E. A. Keiter..... (Harper Collins, 1993)
3. Chemistry of the Elements 2nd ed. - N. N. Greenwood, A. Earnshaw (Butterworth, 1997)
4. Mechanisms of Inorganic Reactions - D. Katakis, G. Gordon (Wiley, 1987)
5. Reaction Mechanism of Inorganic and Organometallic systems, 2nd ed.- R. B. Jordan (Oxford, 1998)

6. Mechanisms of Inorganic Reactions, 2nd ed. - F. Basolo, R.G. Pearson (Wiley, 1967)
7. Inorganic Chemistry- K. F. Purcell, 1C. Kotz (Saunders, 1977).
8. Principles of Organometallic Chemistry, P. Powell, Chapman and Hall; 2nd ed. 1988
9. Basic Organometallic Chemistry, concepts, synthesis and applications, B.D Gupta, A. j Elias, Universities Press; 2nd edition (1 January 2013)
10. Organometallics and Catalysis: An Introduction, OUP Oxford; UK ed. edition 2014.

Course No: MCHMCOC225
Title: Organic Chemistry (04 Credits)

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

Course Objectives:

- To introduce the fundamental principles and applications of spectroscopic techniques viz FTIR, Mass Spectrometry and UV-Visible.
- To introduce the fundamental principles and applications of NMR (1H and 13C) for the structural elucidation of organic compounds.
- To characterize and identify the structure of organic compounds from combined spectral data (FTIR, UV-Vis, ESI-MS and NMR).
- To expose students to the fundamentals of medicinal chemistry.

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

CLO1: understand the fundamental principles and practical applications of spectroscopic techniques such as FTIR, Mass Spectrometry, UV-Vis and NMR for the structural elucidation of organic compounds.
CLO2: interpret spectral data to identify and characterize organic molecules.
CLO3: elucidate the structure of organic compounds using combined (UV, IR, Mass and NMR) spectroscopic methods.
CLO4: understand structure activity and basic concepts of medicinal chemistry in drug design.

Unit-I Ultraviolet Spectroscopy, Infrared Spectroscopy & Mass Spectrometry (15 hours)

Ultra-Violet Spectroscopy: Electronic transitions in organic molecules, Woodward Fieser rules for calculation of λ_{max} of organic compounds.

Infrared spectroscopy: The Infrared spectrum, The functional group and fingerprint regions, Characteristic IR absorption bands, Intensity and position of absorption bands. Structural features that affect vibrational frequency. Application of IR spectroscopy in structural elucidation of organic compounds.

Mass spectrometry: Instrumentation, Determination of molecular formula, Role of Isotopes, Nitrogen Rule. Fragmentation pattern like Stevenson rule, initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels Alder cleavage, Mc-Laffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines.

Unit-II Proton NMR Spectroscopy (15 hours)

Basic concepts, Mechanism of Measurements, Chemical shift values for various classes of compounds. Fourier Transform (FT): techniques and advantages. One bond coupling, two bond coupling, three bond coupling, second order spectra A_2, AB, AX, AB_2, ABX, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange. Nuclear Overhauser Effect (NOE). Applications of ^{1}H NMR in structural elucidation of simple and complex compounds.

Unit-III Carbon-13 NMR spectroscopy (15 hours)

Carbon 13-chemical shifts, proton coupled and decoupled spectra. Off-Resonance De-coupling. DEPT-45, DEPT-90, DEPT-135. NOE signal enhancement. Applications of ^{13}C-NMR in structural elucidation of simple and complex compounds.

Structure elucidation of organic compounds using combined spectroscopic methods (UV, IR, Mass and NMR): Problem based Exercises

Unit-IV Medicinal Chemistry (15 hours)

QSAR and Drug Discovery: Definition and scope of QSAR (Quantitative Structure–Activity Relationship) in drug discovery and medicinal chemistry. Theories of Drug Activity: Clark's Occupancy Theory, Rate Theory, and Two-State Theory. Physicochemical Parameters in Drug Design: Lipophilic constant, Hammett constant, steric parameters, and Hansch analysis. *Psychoactive Drugs:* Introduction to psychoactive drugs; classification: CNS depressants, CNS stimulants, sedatives, and hypnotics. Synthesis of Diazepam, Phenytoin, and Glutethimide. *Cardiovascular Drugs:* Introduction to cardiovascular diseases and related drugs. Synthesis of Amyl Nitrite, Quinidine, Verapamil, Methyldopa, and Atenolol.

Anti-neoplastic drugs: Introduction; cancer chemotherapy, carcenolytic antibiotics, role of alkylating agents and anti-metabolites in treatment of cancer, mitotic inhibitors (elementary idea).

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	2	3	3	3	2	3	2.7
CLO2	2	3	1	3	2	3	2	2.3
CLO3	2	3	1	3	3	3	2	2.4
CLO4	3	3	1	3	2	3	2	2.4
Average PLO	2.5	2.8	1.5	3.0	2.5	2.8	2.3	2.5

Books Recommended:

1. Spectrometric Identification of Organic Compounds. 5th Ed., *R. M. Silverstein,*
2. *G. C. Bassler and T. C. Morill.* (Jhon Wiley) 1991.
3. Introduction to NMR Spectroscopy, *R. J. Abraham. J. Fisher and P. Loftus* (Wiley) 1991
4. Applications of absorption spectroscopy of Organic Compounds, *J. R. Dyer* (Prentice
5. Hall) 1992.
6. Spectroscopic Methods in organic Chemistry, *D. H. Williams; I. Fleming* (Tata- McGraw
7. Hill) 1988.
8. Introduction to Spectroscopy. 5th Edition. *Donald L. Pavia, Gary M. Lampman, George S. Krizand James R. Vyvyan*. 2015
9. Introduction to Medicinal Chemistry, *Alex Gringauz* (Wiley- VCH) 1997
10. Medicinal Chemistry- An Introduction, 3rd Ed., *Gareth Thomas* (Wiley) 2000.
11. Medicinal Chemistry, *Ashutosh Kar*. (Wiley Eastern) 1993.
12. Organic Chemistry by *I. L. Finar Vol. II* (ELBS Longamnn) 1956.

13. Lehninger's Principles of Biochemistry, *D.L. Nelson. M. Cox* Worth publications, 2000

Course No: MCHMCLC225
Title: Laboratory Course in Chemistry-2 (04 Credits)

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

Course Objectives:

- Learn synthetic methodology and correlate synthesis and inorganic reaction mechanism.
- Use titrations as tool to have hands on instruments, instrument handling and experiment designing for evaluation of composition, thermodynamic parameters and reaction monitoring.
- Train students in the separation, purification, and identification of organic compounds from multicomponent mixtures using classical techniques.
- Develop competency in executing key organic reactions and characterizing the synthesized products through crystallization and melting point analysis.
- Understand and apply conductometric techniques for the quantitative analysis of acid-base reactions, mixture compositions, and precipitation processes.
- Impart experimental skills to investigate phase equilibria and solubility behavior in binary and ternary systems, and analyze critical solution temperatures.

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

CLO1: synthesize, analyze and transform coordination and other inorganic compounds.

CLO2: have a comprehensive hand set on the use of potentiometry and other bench level techniques for monitoring experiments, quality control, thermodynamic analysis and comparative analysis.

CLO3: perform systematic separation, purification, and identification of components from an organic mixture using functional group-based techniques.

CLO4: synthesize, purify, and characterize organic compounds through standard reactions (e.g., bromination, amidation, oxidation), and assess product purity using crystallization and melting point determination.

CLO5: perform conductometric titrations to determine dissociation constants, mixture compositions, and concentrations of electrolytes using principles of ionic conductivity.

CLO6: analyze phase diagrams and determine critical solution temperatures by studying the mutual solubility of binary and ternary systems under varying conditions.

SECTION A-INORGANIC CHEMISTRY

A: -Inorganic Preparations: (Any 03 Experiments)

1. • Preparation of tris(ethylenediamine)nickel(II) chloride dihydrate and analysis of stepwise complexation process.
2. Preparation of Potassiumtrisoxalatoferrate(III)trihydrate and its component analysis.
3. Preparation of Pentaamminecholorocobalt(III) chloride and its conversion to nitrito and isomers to study Linkage isomerism by FTIR.
4. Photo redox mediated organic transformation using $[Ru(bipy)_3]Cl_2$ photocatalyst. (Demonstration)

B: - Analytical Titrations: (any 05 Experiments)

1. Potentiometric evaluation of redox descriptors: formal and Transition redox potentials.
2. Comparative thermodynamic analysis of $Fe^{2+}/Cr_2O_7^{2-}$ and Fe^{2+}/ Ce^{4+} redox reactions in acidic medium.
3. Complexation effect on redox potential of iron redox couple and its analytical application.
4. Estimation of Iodide using $I^-\backslash I_2$ redox couple involving pseudo indicator action.
5. Evaluation of reaction stoichiometry between Ferrocyanide and standard Zinc (II) solution and establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$
6. Speciation analysis of the $CrO4^{2-}/ Cr_2O_7^{2-}$ ions in a binary mixture using pH sensitive equilibrium.
7. Investigation of silver(I) ethylenediamine complexation reaction

SECTION B-ORGANIC CHEMISTRY

A. **Organic Preparations (Two stage)**

(a) Bromination of Acetone using Bromine/NBS and PTS
(b) Amidation Reaction
(c) Acetylation Reactions
(d) Haloform reaction: Preparation of Iodoform.
(e) Oxidation of Cyclohexanol by chromic acid to get adipic acid.
(f) Monitoring the progress of reaction and checking the purity of the products using TLC.
(g) Recording the IR of starting material and the products. Identify the changes and reasons thereof.
(h) Crystallization, m.p. determination and Characterization of Synthesized Compounds.

B. **Separation and identification of amino acid from a given mixture using paper chromatography.**

SECTION C-PHYSICAL CHEMISTRY

A. Conductometry

1. Determination of equivalent conductance, degree of dissociation and the dissociation of a weak acid.
2. Determination of the composition of a mixture of HCl and CH_3COOH by titration with standard NaOH.
3. Precipitation titration of $BaCl_2$ and $K_2SO_4/ (NH_4)_2SO_4$
4. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.

B. Phase Equilibria

1. Investigate the mutual solubility of phenol and water at various temperatures and hence determine the critical solution temperature of phenol-water system.
2. Study the effect of addition of NaCl/Succinic acid on the critical solution temperature of Phenol-Water System.
3. Investigate the solubility of three component systems and hence draw a tie line on binodal curve.

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	2	2	3	2.6
CLO3	3	3	3	2	3	3	3	2.9
CLO4	3	3	3	2	2	3	3	2.7
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	2.5	2.7	2.8	2.7

Books Recommended:

1. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, **1992.**)
2. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., **1989).**
3. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, **1999)**.
4. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, • **1996)**
5. Comprehensicve Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-**2000)**
6. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
7. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
8. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.

Course No: MCHMCSP225
Title: Infrared, Raman and Electronic Spectroscopy (02Credits)

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

Course Objectives:

- To introduce the fundamental principles of spectroscopy and explore the interaction between electromagnetic radiation and matter, including concepts such as transition probability and selection rules.
- To develop an understanding of vibrational and rotational spectroscopy, including IR and Raman techniques, their quantum mechanical background, and applications in molecular structure determination.
- To examine electronic and photoelectron spectroscopy, focusing on vibronic transitions, Franck-Condon principle, and molecular electronic transitions and their selection rules.

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

CLO1: describe the principles of electromagnetic radiation interaction with matter, explain spectral line broadening mechanisms, and apply Beer-Lambert Law for quantitative analysis.

CLO2: interpret IR and Raman spectra of diatomic and polyatomic molecules, apply selection rules, and relate vibrational and rotational transitions to molecular structure and bonding.

CLO3: analyze electronic transitions in molecules, including vibronic structures and symmetry considerations, using concepts such as Franck-Condon principle and molecular term symbols.

Unit-I (15 Contact hours)

Fundamentals of Spectroscopy

Interaction of electromagnetic radiation with matter, transition probability, transition dipole moment integral, selection rules, Natural spectral line width and broadening of spectral lines - Doppler and Collision effects. (03 hours)

Intensity of spectral lines, Fourier Transform Spectroscopy.

Beer Lambert Law and its application in determining the concentration of analytes. (03 hours)

Infrared Spectroscopy

Linear-harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration- rotation spectra of diatomic molecules; P, Q and R branches. (7 hours)

Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Group frequencies and finger print region. (2 hours)

Unit-II (15 Contact hours)

Raman Spectroscopy

Classical concept of Raman scattering, molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications. (06 hours)

Electronic and Photoelectron Spectroscopy

Molecular Electronic Spectroscopy: Vibronic transitions, Franck-Condon principle, electronic spectra of polyatomic molecules, Different types of electronic transitions; nomenclature, symmetry labels of electronic states--spectra of formaldehyde, Symmetry selection rules, molecular Term Symbol (Elementary Idea). (06 hours)

Photoelectron Spectroscopy: Basic principles- photoionization process; ionization energies; Koopman's theorem. Photoelectron spectra of simple molecules (N_2, O_2). (03 hours)

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	2	3	3	3	2	2.6
CLO3	2	3	2	3	2	3	2	2.4
Average PLO	2.3	2.7	2.3	3.0	2.7	2.3	2.0	2.5

Books Recommended

1. Molecular Spectroscopy; 2nd edn; J L. McHale; CRC Press 2015.
2. Infrared and Raman Spectroscopy; Principles and Spectral Interpretation; 2nd edn.; P. Larkin; Elsevier; 2011.
3. Introduction of Spectroscopy; 4th edn.; D.L. Pavia, G. M. Lampman, G.S.Kriz,J.Vyvan; Cengage Learning, 2008.
4. Introductory Raman Spectroscopy; J. R. Ferraro, K.Nakamoto& C. W Brown; 2nd edn; Academic Press 2005.
5. Modern Spectroscopy; J.M.Hollas; Wiley; 2004..
6. Physical Methods for Chemists; R.S.Drago; 2nd edn; Saunders; 1992.
7. Fundamentals of Molecular Spectroscopy; C.N.Banwell, E.M.Mc Cash; 4th edn; TataMcGrawHill; 1994.
8. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
9. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; Universities Press.
10. Theory and Applications of Ultraviolet Spectroscopy; H.H.Jaffe, M.Orchin; Wiley; 1962.

11. Molecular Spectroscopy; 1st Edn; J.L. Mchale; Prentice Hall; 1999.
12. Structural Methods in Inorganic Chemistry; 2nd edn; E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock; Blackwell; 1991.

Course No: MCHMCPC225
Title: Organic Photochemistry and Radical Reactions (02 Credits)

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

Course Objectives:

- To provide foundational understanding of photochemistry in organic systems.
- To develop expertise in modern organic synthesis through the study of light-induced reactions.
- To make students acquainted with photochemical reactions of organic nitrites and their synthetic utility (Barton reaction).
- To provide knowledge of radical reactions and their synthetic utility.

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

CLO1: Explain the fundamental principles of photochemistry, including interaction of electromagnetic radiation with matter, excited states (singlet and triplet), and energy transfer processes such as sensitization and quenching.

CLO2: Analyze and predict photochemical reactions of alkenes and dienes. *Evaluate the mechanisms and outcomes of photochemical transformations in carbonyl compounds*, including intramolecular (Norrish Type I and II) and intermolecular reactions (e.g., Paternò–Büchi reaction), as well as unsaturated carbonyl systems and their unique reactivity.

CLO3: Interpret the photochemical behavior of aromatic compounds and apply this knowledge to synthetic and biological contexts, such as photoaddition, nucleophilic photo substitution, Fries rearrangement

CLO4: Understand the formation, structure, and reactivity of free radicals, and apply radical-based substitution and coupling reactions in organic synthesis.

Unit-I Photochemistry-I (15 Contact hours)

Interaction of electromagnetic radiation with matter. Types of excitations. Singlet and triplet states and their lifetimes. Fate of excited molecule: Physical and chemical processes. Transfer of excitation energy: Sensitization and Quenching. Photochemistry of alkenes: Geometrical isomerization's, cyclisation and dimerization reactions. Photochemical reactions of 1,3- butadiene (excluding pericyclic reactions), rearrangements of 1,4 and 1,5- dienes. Photochemistry of saturated carbonyl compounds Intramolecular reactions of saturated acyclic and cyclic carbonyl compounds (Norrish Type I and Norrish Type-II processes). Intermolecular cycloaddition reactions (Paterno- Buchi reaction). Photochemical reactions of α,β- unsaturated carbonyl compounds (H-abstraction and isomerization to β,γ-unsaturated systems). Photolysis of α, β unsaturated cyclic ketones (dimerization and Lumiketone rearrangement) and cyclohexadienones.

Unit-II Photochemistry –II and Radical Reactions (15 Contact hours)

Photochemistry of Aromatic compounds: Photoinduced isomerization of benzene and its alkyl derivatives. 1,2, 1,3 and 1,4 photoaddition reactions of benzene. Nucleophilic photo-substitution reactions in aromatic compounds. Photo Fries-rearrangement of aryl esters.
Miscellaneous photochemical reactions: Barton and Hofmann-Löffler-Freytag reactions and their synthetic utility.
Radical Reactions: Formation, structure and reactivity of free radicals (recapitulation). Electrophilic and nucleophilic radicals. Free radical substitution reactions: Selectivity, stereochemistry and synthetic utility of halogenation of alkane. Neighboring group assistance, bromination using NBS. Coupling reactions: Coupling of alkynes, arylation of aromatic compounds by diazonium salts. Titanium promoted Pinacol coupling (McMurry reaction). Hunsdicker reaction. Autooxidation and antioxidants

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. Introductory Photochemistry, A. Cox and T. Kemp (McGraw Hall) 1971.
2. Organic Photochemistry, 2nd Ed., J. Coxon, and B. Halton (2nd Ed. Cambridge University press) 1987.
3. Fundamentals of photochemistry, Rohatgi & Mukherjee (Wiley Eastern) 1992.
4. Organic Chemistry, 10th Ed.;. T. W. G. Solomons and Craig B. Fryhle ; (Wiley) 2012.
5. Organic Chemistry; 4th Ed., Clayden, Greeves, Warren and Wothers ; (Oxford University Press) 2012.