Course No: MCHMCPC325
Title: Physical Chemistry (04 Credits)

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

Course Objectives:

- To develop an advanced understanding of chemical bonding through molecular orbital and valence bond theories, with emphasis on multi-electron systems and self-consistent field methods.
- To introduce and apply statistical mechanics principles to molecular systems and derive thermodynamic properties using partition functions.
- To explain the structure and dynamics at electrified interfaces, including the theoretical background of electron transfer and corrosion phenomena.
- To explore the principles, types, and mechanisms of catalysis with emphasis on modern catalytic processes and green chemistry approaches.
- To equip students with quantitative tools and models to analyze physicochemical systems at the quantum, statistical, and electrochemical levels.
- To integrate concepts of quantum chemistry, statistical mechanics, electrochemistry, and catalysis to solve real-world problems in industrial and research contexts.

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

CLO1: Analyze molecular systems using LCAO-MO and VB approaches and compare their predictions for bonding and stability in diatomic and polyatomic systems.

CLO2: Apply Huckel theory to linear and cyclic conjugated systems and evaluate molecular properties such as bond order and electron distribution.

CLO3: Derive and interpret the statistical distribution laws (Boltzmann, Fermi-Dirac, Bose-Einstein) and apply them to calculate thermodynamic properties.

CLO4: Evaluate electrochemical phenomena at metal-electrolyte interfaces using models like Gouy-Chapman and Butler-Volmer theory.

CLO5: Explain catalytic mechanisms, including metal-catalyzed reactions and the role of solvents and hydrophobic interactions in rate enhancement and selectivity.

CLO6: Critically assess industrial catalytic processes such as Fischer-Tropsch synthesis and ammonia production from a mechanistic and kinetic perspective.

Unit-I Quantum Chemistry-3 (15 Contact hours)

Chemical Bonding: LCAO-MO approximation, H_2^+ molecular ion, brief introduction to H_2. Valence bond treatment of hydrogen molecule, comparison of MO and VB methods in the light of hydrogen molecule. Hybridization of orbitals (sp, sp^2 & sp^3). Huckel's Pi-MO theory: Application to linear and cyclic polyenes. Pi-electron charge and bond-order. Alternant hydrocarbons, heteroatomic conjugated systems. Limitations of Huckel theory.

Self consistent field method: Hamiltonian and wave function for multi-electron systems (antisymmetrized wave function), and Slater determinant. Hartree and Hartree-Fock self consistent field method. Application of Hatree Fock SCF method to He- atom.

Unit-II Statistical Mechanics (15 Contact hours)

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi- Dirac laws and their comparison with Boltzmann distribution law.
Partition function & its significance. Translational, rotational, vibrational and electronic partition functions. Relation between partition function and thermodynamic functions. Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic & diatomic gases.
Applications of distribution laws: Distribution of molecular velocities in ideal gases, Black body radiations, electron gas in metals, Bose-Einstein condensation.
Statistical mechanics of solids: Einstein and Debye models (Partition function, average energy and heat capacity), and their limitations.

Unit-III Electrochemistry-2 (15 Contact hours)

Electrified Interface: Metal-electrolyte electrified interface, concept of surface excess, thermodynamics of electrified interface, Lippman equation, electrocapillary curves. Methods for determination of surface excess.
Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, Structure of semiconductor/electrolyte interface.
Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butler-Volmer equation, low and high field approximations, significance of transfer coefficient, Marcus theory of charge transfer; basics and predictions.
Electrodics of Corrosion: Corrosion, types and mechanism of corrosion, corrosion current, corrosion potential, Electrodics of corrosion in absence of Oxide films, Corrosion and Evans diagrams, Monitoring and inhibition of corrosion; Cathodic and anodic protection, Passivation.

Unit-IV Advanced Catalysis (15 Contact hours)

Catalysis the Basics: Catalysis and green chemistry, homogeneous, heterogeneous and bio-catalysis, Catalytic cycles, Turn over number, Turn over frequency, Catalyst deactivation, sintering, thermal degradation, Inhibition, poisoning. Replacing Stoichiometric Reactions with Catalytic Cycles.
Potential functions of catalysts with examples; reaction initiation, intermediate/transition state stabilization (Sabatier's principle), reactant localization and reactant orientation, bond cleavage facilitation, electronic effect, reaction selectivity enhancement, energy and mass transfer facilitation effects of catalysts.
Solvents as catalysts: solvation and its impact on reactant, product and transition state stabilization, impact of solvent on reaction rates, qualitative and semiquantitative predictions of the effect of solvents on reaction rates. Hydrophobic interactions, examples regarding facilitation of reaction kinetics and reaction selectivity via use of hydrophobic interactions.
Catalysis by Metals: Elementary reactions on metals, mechanism of metal catalyzed reactions, Blowers-Masel equation for catalyst selection.
Catalysis of Industrial processes: Mechanistic and kinetic aspects of some selected industrial process; Synthesis Gas, Synthesis of methanol, Fischer-Tropsch process, Synthesis of ammonia.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	2	3	3	2	3	2.7
CLO2	3	2	2	3	2	3	3	2.6
CLO3	3	3	3	3	3	2	2	2.7
CLO4	2	3	3	3	3	3	2	2.7
CLO5	3	3	3	2	2	2	2	2.4
CLO6	2	2	2	2	1	3	3	2.1
Average PLO	2.7	2.7	2.5	2.7	2.3	2.5	2.5	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. Statistical Thermodynamics, M. C. Gupta, New Age International, 1993.
8. Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.
9. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
10. Statistical Thermodynamics, Andrew Maczek, Anthony Meijer, Oxford University Press 2023.
11. Modern Electrochemistry 1, 2A, 2B 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
12. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley,1980.
13. Physical Electrochemistry- Fundamentals, Techniques and Applications, Eliezer Gileadi, Wiley-VCH 2011.
14. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
15. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
16. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.
17. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola,New York, 2001.
18. Introduction To Heterogeneous Catalysis, Roel Prins, Anjie Wang, Xiang Li , World Scientific Publishing Company, 2016.
19. Catalysis, Concepts and Green Applications, Gadi Rothenberg, Wiley, 2017.
20. Concepts of Modern Catalysis and Kinetics, I. Chorkendorff, J. W. Niemantsverdriet, Wiley 2006.
21. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001.

Course No: MCHMCIC325
Title: Inorganic Chemistry (04 Credits)

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

Course Objectives:

- To analyze how metal–ligand bonding modes govern reactivity patterns across different organometallic families.
- Understand design, mechanisms, and applications of homogeneous transition metal catalysts in organic synthesis.
- To evaluate dynamic (fluxional) behavior of complexes and reconcile NMR, X-ray, and other structural snapshots obtained at different time scales.
- To apply Schrock- and Fischer-carbene chemistry as building blocks ("synthons") in
- homogeneous catalysis.
- To interpret magnetic measurements and magneto-structural correlations to characterize single-molecule magnets (SMMs) and other transition-metal complexes.
- To utilize advanced spectroscopies (Mössbauer, NQR) to probe Fe and Sn compounds and understand light- vs. dark-driven reactivity.
- To understand role and working of metal ion based biomolecules for bio functioning and therapeutics.

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

CLO1: analyze metal–ligand bonding and correlate it with the reactivity of diverse organometallic complexes.
CLO2: design catalysts for olefin metathesis, C-C coupling, and photoredox reactions; analyze oxidative addition/insertion mechanisms.
CLO3: apply the concepts of Schrock and Fischer carbenes in designing catalytic processes.
CLO4: interpret magnetic and magneto-structural data to characterize transition metal complexes and single-molecule magnets.
CLO5: utilize Mössbauer and NQR spectroscopy to investigate the structure and reactivity of Fe/Sn compounds.
CLO6: understand chelation therapy parameters using PMI, HSAB theory, and conditional stability constants.

Unit –I Organometallics --- I (15 Contact Hours)

Designing of a homogenous Transition Metal catalyst. Mechanistic aspects (Oxidative addition, Insertion reaction and water gas shift reaction). Olefin homogenous catalysis: Oxidation, Isomerization, metathesis and Ziegler Natta polymerization. Carbon-Carbon coupling reactions (Suzuki and Heck)
Schrock and Fischer carbene complexes: Structural characteristics; reactivities and synthetic applications(Dotz reaction and Schrock's Catalyst).
Activation of small molecules: prospectus and challenges. Selected reactivities of coordinated ligands: carbon monoxide, alkanes and alkenes (Green, Mingo's rules). Photoredox catalysis in organic transformations . Role of organo-iron compounds as synthons.

Unit-II Magnetic and Electronic Properties of Transition Metal Complexes (15 Contact Hours)

Magnetic interaction in dinuclear and polynuclear clusters (examples) magnetic susceptibility: determination, temperature dependence. Magnetic moment; spin-only formula; correlation of μs and μeff values; orbital contribution , magnetic properties with A, E and T ground terms, applications of magnetic moment data in evaluation of nature and complexation parameters. High spin-low spin crossover. Introduction to single molecule magnets (SMMs) and related applications, Magnetic properties of inner transition compounds.Importance of computational approaches in predicting the magnetic behavior of metal complexes.Hands-on training to data analysis: magneto-structural correlations and PHI software).

Types of electronic transitions in metal complexes, selection rules and their relaxation mechanisms; spectral terms of d^1 - d^{10} metal ions. Selected examples of d-d spectra. Orgel diagrams, Charge transfer spectra (Factors affecting energies of LMCT and MLCT transitions).

Unit-III Mossbauer and NQR Spectroscopy. (15 Contact Hours)

Mossbauer Spectroscopy: Basic principles, Nuclear Recoil and Mossbauer Effect, Spectral parameters such as isomer shift, quadrupole splitting and magnetic splitting, spectrum display. Determination of Magnetic transition Temperature, Intermediate spin -- Determination of Spin crossover temperatures. Partial Isomer shift and partial Quadrupole splitting. Application of the technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds (ii) Sn^{2+} and Sn^{4+} compounds— nature of M—L bond, coordination number and structure, (iii) detection of oxidation state and inequivalent MB atoms. (b)

NQR Spectroscopy: NQR isotopes, Nuclear quadruple moment; Electric field gradient; nuclear quadruple coupling constant; Axial Symmetry, Asymmetric EFG, Effect of applied magnetic field, Applications.

Unit-IV : Bio coordination chemistry (15 Contact hours)

Metalloporphyrins: General concept, structural characterization and biological functioning in O2 transport, electron transport and activation of small molecules.
Metalloenzymes: Active site structure and mechanistic details of Catalase and Carbonic anhydrase. **Metal based therapeutics:** Structure activity response of Pt^{II} and Ru^{II} based anticancer drugs. Metal based radiopharmaceuticals, Metal complex as enzymes modulators.
Chelation therapy: Types of Chelation Therapy: Single, Double, Synergistic and Mixed ligand chelation therapy. Therapeutic index of different chelating drugs in metal ion detoxification. Limitations and Hazards of Chelation therapy.
Therapeutic Aspects of Chelating Drugs: Conditional stability constant, Stereochemistry, Lipophilicity. HSAB theory and Plasma mobilizing index (PMI).

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	2	2	3	3	3	3	2.7
CLO3	2	3	3	3	3	2	2	2.6
CLO4	2	3	3	3	3	3	2	2.7
CLO5	3	3	3	2	2	2	2	2.4
CLO6	2	2	2	2	1	3	3	2.1
Average PLO	2.5	2.7	2.7	2.7	2.5	2.7	2.5	2.6

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 6th edn; Robert. H . Crabtree; Wiley;2014.
2. 2. Fundamental Transition Metal Organometallic Chemistry; Charles M. Lukehart; Brooks / Cole;1985.
3. Basic Organometallic Chemistry; 2nd edn ; Gupta Elias ; CRC Press, 2010
4. Principles and Applications of Organotransition Metal Chemistry; Collman& Finke; University, Science Books; 1994.
5. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall; 1998
6. Elements of Magnetochemistry; R. L. Dutta, A. Syamal; Affiliated East-West;1993.
7. Electronic Spectra of Transition Metal Complexes; D. Sutton; McGraw-Hill; 1968.
8. NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish; EllisHorwood; 1990.
9. Spectroscopy in Inorganic Chemistry; Vol I & II; Rao, Ferraro; Academic Press; 1970.
10. Physical Methods for Chemistry; 2nd edn.; R .S. Drago; Saunders; 1992.
11. Principles and Applications of Photochemistry, B. Wardle, John Wiley, 2009
12. Ligand Field Theory and Its Applications; B. A. Figgis and M. A. Hitchman; Wiley India,2000.
13. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.;Jordon; Oxford; 1998.
14. Inorganic Chemistry; G. Wulfsberg; Viva Books, 2000.
15. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
16. Inorganic Chemistry, Principles of structure and reactivity; 4th edn; J. E. Huheey,E. A. Keiter and R. L.Keiter. Pearson Education Inc.2003
17. Biomedical Applications of Inorganic Photochemistry, Peter C. Ford, Rudi van Eldik 1st Edition, Volume 80 – 2022 , Academic Press Hardback ISBN: 9780323991711.
18. A Textbook of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
19. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991.
20. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books;1994.
21. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.

Course No: MCHMCOC325
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 deep knowledge about various reagents used in organic synthesis.
- To develop understanding and synthetic utility of organometallic reagents.
- To develop the understanding of asymmetric synthesis and different methods of stereoselective synthesis.
- To give an idea about the biosynthesis of Natural Products and role of steroidal hormones.

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

CLO1: Understand and apply various oxidizing, reducing, and specialized reagents in organic synthesis.

CLO2: Analyze and perform C–C bond formation using organometallic reagent and palladium-catalyzed coupling reactions.

CLO3: Understand the intricacies of asymmetric synthesis and stereochemical control in synthesis of complex organic molecules.

CLO4: Describe and evaluate the structure, biosynthesis, chemical properties and biological function of Natural Products.

Unit-I Reagents in Organic Synthesis (15 Contact hours)

Oxidizing Reagents:
meta-Chloroperoxybenzoic acid (MCPBA), N-Chlorosuccinimide (NCS), Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC), tert-Butyl hydroperoxide (TBHP), 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), Manganese dioxide (MnO_2), 2,2,6,6-Tetramethylpiperidine 1-oxyl (TEMPO), Ceric Ammonium Nitrate (CAN), Thallium Nitrate.

Reducing Reagents:
Sodium borohydride ($NaBH_4$), Diisobutylaluminum hydride (DIBAL), Lithium aluminum hydride (LAH), Diisoamylborane, Lindlar's catalyst ($Pd/BaSO_4$) Sodium in ethanol-dissolving metal reduction (Na/EtOH), Na/liquid NH_3 (Birch reduction).

Specialized Reagents:
Dicyclohexylcarbodiimide (DCC), 1,4-Diazabicyclo [2.2.2] octane (DABCO), 1,8-Diazabicyclo [5.4.0] undec-7-ene (DBU).

Unit-II Formation of Carbon-Carbon Bond via Organometallic Reagents (15 contact hrs)

Organolithium Reagents: Preparation, aryllithium reagents, reactions, and chemoselectivity.
Organomagnesium Reagents: Preparation of Grignard reagents, reactions with carbonyl compounds, and limitations.
Organocopper Reagents: Preparation and reactions of organocuprates.
Organozinc Reagents: Preparation and reactions of organozinc compounds.
Palladium-Catalyzed Coupling Reactions: Suzuki, Heck, Negishi, Stille, Sonogashira, and Trost–Tsuji reactions.

Unit-III Asymmetric Synthesis (15 Contact hours)

Nature & asymmetry, Chiral pool approach, Chiral auxiliaries and auxiliary controlled stereo-selection. Chiral reagents. Asymmetric formation of C-C bonds: Asymmetric aldol and Baylis-Hillman reactions. Asymmetric hydrogenation and epoxidation of alkenes (Sharpless, Jacobsen and Shi reactions). Racemization & Resolution of enantiomers using chiral molecules. Stereoselectivity: Stereochemical control in six-membered rings, Stereoselectivity in bicyclic compounds.

Unit-IV Advanced Natural Products Chemistry (15 Contact hours)

Flavonoids: Occurrence, isolation and classification. Structure determination and synthesis of Chrysin, Quercetin, Genistein, and Cyanidin. Antioxidant activity of flavonoids. Biosynthesis of Flavonoids (Acetate and Shikimic acid pathways).
Alkaloids: Chemistry of Nicotine, Quinine and Morphine: Biosynthesis of Quinine
Steroids: Structure and biological role of Sex-hormones **(**Oesterone, Testosterone, androsterone and Progesterone**).** Corticosterioiods: (Cortisone) and Vitamin D.

CLO-PLO Mapping Matrix (Strength version)

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

Books Recommended

1. Modern Methods of Organic Synthesis, *Carruthers W. William Caruther and Iain Coldham*, 4th edition, Cambridge, 2024.
2. A Guide to Reagents in Organic Synthesis., *S Gupta, V Gupta, R.S Dhundal*, 1st edition, 2015
3. Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, by *Jiro Tsuji*, 2002.
4. Advanced Organic Chemistry Part B, 5th edn.*; F. A. Carey and R.J Sundberg*; Springer; 2007.
5. Organic Chemistry; 4th Ed., *Clayden, Greeves, Warren and Wothers* ; Oxford University Press-2012.
6. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6lh Ed., *J. March*,; Wiley; 2012
7. Stereoselectivity in Organic Synthesis, Garry Procter, Oxford University Press, 1996.
8. Principles of Asymmetric Synthesis, *Robert E. Gawley and Jeffery Aube*, 2nd Edition, 2012.
9. Stereochemistry of Organic Compounds, *V.K. Ahluwalia*, Springer, 2022.
10. Principles and Applications of Stereochemistry, *Michael North*, CRC Press-1998.
11. Stereochemistry and Stereoselective synthesis: An Introduction, *Laszlo Poppe and Mihaly Nogardi,* Wiley-VCH, 2016.
12. Chemistry of Natural Products; *S. V. Bhat, B. A. Nagasampagin*. (Narosa 2005).
13. Organic Chemistry, 5th Ed. Vol.2,*I. L. Finar* (Addison Wisley Longman-2000).
14. Chemistry of Natural Products, *N.R. Krishnaswamy* (University Press-1999).

Course No: MCHMCOS325
Title: Designing Organic Synthesis (02 Credits)

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

Course Objectives:

- To impart knowledge on the strategic use of functional group protection in organic synthesis.
- To elucidate the interconversion and retrosynthetic analysis in organic synthesis.
- To develop the understanding for designing efficient synthetic pathways for complex organic molecules.

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

CLO1: Understand and apply the principles of protection and deprotection of functional groups in organic synthesis to selectively modify complex molecules.
CLO2: Analyze and perform functional group interconversions (FGIs) with an emphasis on chemoselectivity and strategic planning in synthetic routes.
CLO3: Demonstrate proficiency in the disconnection approach for organic synthesis by identifying appropriate synthons, applying polarity inversion and executing one-group and two-group disconnections.
CLO4: Design multi-step synthetic routes for complex organic molecules using retrosynthetic analysis, incorporating both functional group transformations and disconnection strategies.

Unit-I Protection and Interconversion of Functional Groups (15 Contact hours)

Protection of functional groups: Principle of protection of functional groups and its significance. Protection of carbon-carbon double bonds, alcoholic and phenolic hydroxyl groups, amino groups, carbonyl and carboxyl groups. Protection of carbon-hydrogen bonds (in terminal alkynes and α carbon-hydrogen bond of aldehydes and ketones).

Functional Group Interconversion (FGI) / Transformations: Significance of Functional Group

Interconversion (FGI)/Transformations in Organic synthesis. Methods of transformation ofdifferent functional groups into one another. Chemoselectivity

Unit-II Rational Approaches to Organic Synthesis (15 Contact hours)

The disconnection approach: Introduction to synthons, their types and equivalent reagents.
Reversal of Polarity(umpolung). One group, two group and Reteroelectrocyclic. disconnections. Reterosynthetic Analysis involving connections and rearrangements.Guidelines for good disconnections.
One group disconnections: Reterosynthetic analysis of alcohols, amines (aliphatic andaromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using onegroup disconnections and FGIs. Use of acetylenes in the syntheses of above mentionedcompounds.
Two group disconnections: Reterosynthetic analysis of 1, 2- difunctional compounds (1,2 –diols), 1,3-difunctional compounds (1,3-dioxygenated compounds, α, β-unsaturated carbonylcompounds, 3-amino alcohols and 3- amino ketones), 1,4- and 1,5-difunctional compounds.Multistep Synthesis: Application

of reterosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benziodarone, Juvabione, warfarin and brevicomin (Examples other than these may also be included).

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	2	3	1	3	2	3	1	2.1
CLO2	2	3	1	3	3	3	2	2.4
CLO3	2	2	1	3	2	3	2	2.1
CLO4	2	3	2	3	2	3	1	2.3
Average PLO	2.0	2.8	1.3	3.0	2.3	3.0	1.5	2.3

Books Recommended

1. Designing Organic Synthesis, *S. Warren*; Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, *J. Furhop and G. Penzlin*; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd Ed., *R. O. C. Norman*; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.*; F. A. Carey and R.J Sundberg*; Springer; 2007.
5. Organic Chemistry, 10th edn;. *T. W. G. Solomons and Craig B. Fryhle* ; Wiley-2012.
6. Organic Chemistry; 4th Ed., *Clayden, Greeves, Warren and Wothers* ; Oxford University Press-2012.
7. March's Advanced Organic Chemistry 6th Ed., *Michael B. Smith & Jerry March,* (Wiley) 2014.

Course No: MCHMCNE325
Title: NMR and ESR Spectroscopy (02 Credits)

Max. Marks: 50 | **Duration: 30 Contact hours**

Continuous Assessment: 14 marks | **End Term Exam: 36 Marks**

Course Objectives:

- To impart foundational understanding of nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy, including quantum mechanical principles governing nuclear and electron spins.
- To explore and analyze factors influencing spectral parameters such as chemical shift, spin-spin coupling, relaxation, hyperfine interaction, and magnetic anisotropy.
- To familiarize students with modern spectroscopic instrumentation and the interpretation of 1H, 13C, 19F, 31P NMR and ESR spectra in both organic and inorganic systems..

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

CLO1: explain the basic principles of NMR and ESR spectroscopy, including energy level splitting, relaxation processes, and resonance phenomena..

CLO2: Analyze NMR and ESR spectral data to interpret chemical shifts, coupling constants, spin densities, and magnetic interactions in various molecular systems.

CLO3: Apply double resonance techniques and advanced spectroscopic methods to characterize nuclei and unpaired electron systems using FT-NMR and ESR instrumentation.

Unit-I: NMR Spectroscopy (15 Contact hours)

Basic principles: Nuclear spin, spin angular momentum, nuclear magnetic moment, precessional (Larmor) frequency, energy levels in a magnetic field, resonance absorption of radio frequency radiation, population of energy levels, Relaxation processes (T1, and T2).

Shielding and deshielding of magnetic nuclei, Chemical shift and factors affecting chemical shifts: local paramagnetic and diamagnetic shielding, neighboring group anisotropy and ring currents in aromatic systems, Spin- Spin coupling, coupling constants and factors influencing coupling constants.

Double resonance techniques; spin decoupling, nuclear Overhauser enhancement. Instrumentation; FT-NMR and its advantages. NMR studies of nuclei other than proton – 13C, 19F and 31P.

Unit-II ESR Spectroscopy (15 Contact hours)

Basic principles- electron spin, magnetic moment of an electron and its interaction with applied magnetic field. Splitting of spin energy states and absorption of microwave radiation.

Hyperfine coupling, Isotropic and anisotropic hyperfine coupling constants, Examples, Fermi contact, Spin polarization effects, Dipolar coupling, Mc Conell equation and calculation of spin densities in inorganic radicals such as CO_2-•, CH_3 •, BH_3-• and F_2-•.

Spin orbit coupling and significance of g tensors. Zero field splitting and Kramer's degeneracy (fine structure), Advance Applications.

CLO-PLO Mapping Matrix (Strength version)

CLO/PLO	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	Average CLO
CLO1	3	3	2	3	2	3	3	2.7
CLO2	3	3	2	3	3	3	2	2.7
CLO3	3	2	2	3	2	3	3	2.6
Average PLO	3.0	2.7	2.0	3.0	2.3	3.0	2.7	2.7

Books Recommended

1. Introduction to Electron Spin Resonance; H. M. Assenheim; Springer, 2014.
2. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR; 2nd edn.; D.N. Sathyanarayana; I K International Publishing House,2013.
3. Understanding NMR Spectroscopy; 2nd edn.; J. Keeler; Wiley-Blackwell;2010.
4. Introduction to Spectroscopy; 4th edn.; D. L. Pavia, G. M. Lampman, G. S. Kriz, J. Vyvyan; Cengage Learning, 2008.
5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R. V. Parish;Ellis Horwood; 1990.
6. Nuclear Magnetic Resonance; P. J. Hore; Oxford;1995.
7. Nuclear Magnetic Resonance Spectroscopy; A physicochemical View; R. K. Harris;Pitman Publishing1983,
8. Principles of Instrumental Analysis; 4th edn.; D. A. Skoog, J. J. Leary; Saunders;1992.
9. Physical Methods for Chemists; 2nd edn.; R. S. Drago; Saunders;1992.
10. Basic Principles of Spectroscopy; R. Chang; McGraw Hill;1971.
11. Introduction to Magnetic Resonance; A Carrington, A. D. McLachlan; Harper & Row;1967.
12. NMR and Chemistry; 2nd edn.; J. W. Akitt; Chapman and Hall;1983.

Course No: MCHMCLC325
Title: Laboratory Course in Chemistry-3 (04 Credits)

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

Course Objectives:

- To develop a conceptual understanding of spectrophotometry and its applications in analyzing electronic effects, composition, and binding in coordination complexes.
- To apply spectrophotometric techniques for kinetic analysis and optical band gap determination of semiconductor and coordination systems.
- To provide hands-on training in separation of inorganic ions using column chromatography techniques followed by quantitative estimation through titrimetric methods.
- To provide hands-on experience in multistep organic synthesis, including classical and microwave-assisted reactions, along with functional group transformations and drug synthesis
- To develop skills in compound purification (chromatography), natural product extraction, and spectral characterization of synthesized or isolated organic compounds.
- To develop students' proficiency in electroanalytical techniques such as potentiometry and pH-metry for the quantitative and qualitative analysis of acids, bases, salts, and redox systems.
- To train students in the application of spectrophotometric methods for analyzing binary mixtures, complex formation, and titrimetric reactions involving transition metal ions.

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

CLO1:perform chromatographic separation of metal ions and accurately estimate their concentrations using permanganometry and complexometric titrations.

CLO2: design spectrophotometric experiment for any targeted problem like quality control, food adulteration, water testing etc

CLO3: analyze and interpret spectral plots for research problems like characterization, calculation of binding and rate constants. Evaluation of semi conductor materials towards design and development of photocatalysts.

CLO4: synthesize pharmaceutically and industrially relevant organic compounds through classical and multistep synthetic methods, and evaluate reaction mechanisms.

CLO5: apply chromatographic and spectroscopic techniques to purify, isolate, and characterize organic and natural products

CLO6: perform potentiometric and pH-metric titrations to determine pKa values, redox potentials, and the extent of hydrolysis in acid-base and redox systems.

CLO7: apply spectrophotometric techniques to quantify components in binary mixtures, carry out titrations, and analyze complexation behavior in coordination systems.

SECTION A-INORGANIC CHEMISTRY

A. Separation by Column Chromatography and Estimations:

1. Separation of permanganate and dichromate ions on Alumina column and followed by estimation by Permanganometry
2. Separation of Cobalt (II) and Nickel (II) on an anion exchange column followed by estimation through EDTA back titrations.

B. Spectrophotometry:

1. Spectrophotometric evaluation of electronic factors influencing optical parameters of selected iron complexes.
2. Comparative study of d^8 octahedral complexes $\{[Ni(phen)_3]^{2+}$ and $[Ni(OH_2)_6]^{2+}\}$ for d-d band analysis and complexation effect on d-d bands.
3. Composition analysis of Fe^{2+} and bipyridyl complexation by Jobs and Molar ratio method analysis.
4. Formula verification of synthesized Potassium trisoxalatoferrate(III)trihydrate spectrophotometrically
5. Rate of dissociation of tris 1,10 phenanthroline nickel (II) complex in acid medium.
6. Band gap evaluation of synthesized (bottom-up approach) silver nano particle spectrophotometrically.

SECTION B-ORGANIC CHEMISTRY

A. Multistep Organic Preparations (Synthesis)

(1) Synthesis of local anesthetics
(2) Synthesis of analgesics.
(3) Synthesis of sulpha drugs
(4) Synthesis using microwaves: Alkylation of diethyl malonate with benzoyl chloride.
(5) Skraup synthesis: Preparation of quinoline from aniline.
(6) Beckmann rearrangement.
(7) Aldol condensation: Dibenzal acetone from acetone and benzaldehyde.
(8) Cannizarro's reaction of 4-Chlorobenzaldelyde.
(9) Aromatic electrophilic substitutions in benzoic acid or aniline.

Monitoring the progress of reaction using Thin Layer Chromatography

B. Extraction of Natural Products

(a) Caffeine from Tea leaves
(b) Lycopene and beta carotene from tomato
(c) Citric acid from lemon juice
(d) Keratin form human hair.

C. Column Chromatography

Monitoring the reaction progress and purity of the products .

D. Spectral Analysis of synthesized/Isolated Compounds

SECTION C-PHYSICAL CHEMISTRY

A. Potentiometry

1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
2. Titration of Fe (II) vs. $K_2Cr_2O_7$ and determination of standard redox potential of Fe^{2+}/Fe^{3+}.
3. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$.

B. pH-metry

1. Determination of pKa values of a tribasic acid by titration with an alkali.
2. Determination of H_3PO_4 content in a given sample of Coca-Cola.
3. Determination of degree of hydrolysis of a given salt using pH-metry.

C. Spectrophotometry

1. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$ or Cobalt (II) and Nickel (II) ions.
2. Spectrophotometric titration of Fe(II) vs. $KMNO_4$.
3. To study the complexation reaction between Fe(III) & salicylic acid.
4. Recording Absorption spectra of a series of conjugated dyes-Application of the particle in one dimensional box. (Optional)

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
CLO7	3	2	3	2	3	3	2	2.6
Average PLO	3.0	2.9	2.6	2.6	2.9	2.7	2.7	2.8

Books Recommended:

1. Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education2002
2. Modern Analytical Chemistry, David HarveyMc Graw Hill.US
3. Analytical Chemistry. 7th edition , Gary D. Christian, Purnendu K. (Sandy) Dasgupta, Kevin A. Schug, Wiley
4. Experiments and Techniques in Organic Chemistry - D. Pasto, C. Johnson and M. Miller (Prentice-hall, 1992.)
5. Microscale and Macroscale Organic Experiments- K.L. Williamson (D.C. Heath and Co., 1989).
6. Advanced Practical Organic Chemistry, 2nd ed. - N.K. Vishnoi (Vikas, 1999).
7. Vogel's Textbook of Practical Organic Chemistry, 5th ed.- A.R. Tatchell (ELBS, • 1996)
8. Comprehensicve Practical Organic Chemistry, V. K. Ahluwalia and Renu Aggarwal, (University Press-2000)
9. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
10. Advanced Practical Physical Chemistry, Yadav , Goel Pub, 1994.
11. Experiments in Physical Chemistry, 5th ed., Schoemaker et al. , MGH, 1989.