MAA PATESWARI UNIVERSITY BALRAMPUR

TWO YEARS

M.Sc. CHEMISTRY Program

Syllabus
(For the Academic Session-2025 onwards)

Maa Pateswari University Balrampur

M.Sc. Chemistry Syllabus

Semester-wise Titles of the Papers in M.Sc. Chemistry and its Content

Year	Sem.	Code	Papers	Credit	Total Credit
I	I		**Paper I:** Spectroscopy I	4	20
			Paper II: Physical Chemistry (Chemical Kinetics and Classical Thermodynamics)	4	
			Paper III: Inorganic Chemistry (Chemistry of Main Group Elements)	4	
			Paper IV: Organic Chemistry (Organic Reaction Mechanism)	4	
			Paper V: Practical	4	
	II		**Paper I:** Analytical Chemistry	4	20
			Paper II: Physical Chemistry (Advanced Quantum Mechanism)	4	
			Paper III: Inorganic Chemistry (Chemistry of Transition Metals)	4	
			Paper IV: Organic Chemistry (Stereochemistry and Pericyclic Reactions)	4	
			Paper V: Practical	4	
II	III		**Paper I:** Select Topics in Chemistry	4	20
			Paper II: Physical Chemistry OR Inorganic Chemistry OR Organic Chemistry	4	
			Paper III: Physical Chemistry OR Inorganic Chemistry OR Organic Chemistry	4	

			Paper IV: Practical	4	
			Paper V: Dissertation	4	
	IV		**Paper I:** Spectroscopy-II	4	20
			Paper II: Physical Chemistry OR Inorganic Chemistry OR Organic Chemistry	4	
			Paper III: Physical Chemistry OR Inorganic Chemistry OR Organic Chemistry	4	
			Paper IV: Practical	4	
			Paper V: Dissertation	4	

Passing Marks: 40% for major/minor/Vocational/Co-Curricular

Marking Distribution out of 100: - 25 Marks for internal Assessment +25 Marks External Practical Exam+ 50 Marks for theory paper.

Purpose of the Program

The purpose of the postgraduate chemistry program at the university and college level is to provide the key knowledge base and laboratory resources to prepare students for careers as professionals in various industries and research institutions.

Program's Outcomes

1. Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in analytical, Inorganic, Organic and Physical Chemistries.
2. Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.
3. Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
4. Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.
5. Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.
6. Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.
7. Students will be able to function as a member of an interdisciplinary problem-solving team.

Evaluation of theory paper

Each theory and practical paper have 100 marks

i. **Internal 25 marks** (10 marks of a written test, 10 marks of assignment and 5 marks for the student attendance and performance).
ii. **Theory exam 75 marks.**

Pattern of paper

1. Paper contains 5 questions of 15 marks each. Time of exam will be 3 hours.
2. Question no 1 is compulsory and divided into 5 parts (such as a, b, c, d and e) each is 3 marks.

3. Question No 2 and 3 will be the long question and have 15 marks each.
4. Question no 4 and 5 divided into two parts (such as a and b) & each is 7 and 8 marks.

Evaluation of Practical paper

i. **Internal 25 marks** (10 marks of a written test, 10 marks of assignment and 5 marks for the student attendance and performance).

ii. Practical exam 75 marks

1. Practical Time: 6h
2. 3 Practical will be done in two days.
3. Each practical will be 15 marks
4. Viva-voce will be 20 marks.
5. Practical record will be 10 marks.

Evaluation of Project paper

1. On the basis of research project done in both semesters, the prepared project report/ dissertation will be evaluated by external and internal examiners in 50 marks separately. The student will be evaluated for 25 marks on the basis of concerned viva voce from his/her research project.
2. Remaining 25 marks will be awarded to the student only when he will publish his research paper related to his/her research project in UGC care listed journal

Suggested Continuous Evaluation Methods:	
Assessment and presentation of Assignment/ Research Orientation assignment	(10 marks)
04 Unit tests (Objective): Max marks of each unit test—10 (average of all four-unit tests)	(10 marks)
Overall performance throughout the semester (Discipline, participation in different activities)	(05 marks)

Maa Pateswari University Balrampur

M.Sc. I Semester		
Paper I		**MCHT-101**
Spectroscopy- I		
Objective: The objective of the course is to help students understand the theoretical aspects of various spectroscopic techniques like UV-Visible, IR, NMR and Mass, which in turn, will enhance their capability of interpreting the spectral data obtained from various techniques and use it for structural elucidation of organic compounds. **Outcome:** Students acquire the knowledge of the instrumentation and principle involved in various advanced spectroscopic and will be able to interpret the spectral data for structural elucidation of organic compounds.		
Unit I	**UV-Visible Spectroscopy:** Different type of electronic transitions, Lambert's Beer's law, Chromophores, Auxochromes, Solvent effect, Red-shift and blue-shift, Woodward's rule for conjugated cyclic and acyclic dienes and α, β – unsaturated carbonyl compounds, Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene), Problems related UV-Visible Spectroscopy	
Unit II	**Infrared Spectroscopy:** Review of linear harmonic oscillator, Vibrational energies of diatomic molecules, Zero-point energy, Force constant and bond strength, Anharmonicity, Morse potential energy diagram, Vibration rotation spectroscopy, P, Q, R branches, Breakdown of Born-Oppenheimer approximation, Selection rules, Overtones, Hot Bands, Absorption by common functional groups, Brief description of IR and F.T.I.R. instruments, Problems related I.R. Spectroscopy	
Unit III	**Raman Spectroscopy:** Theories of Raman Effect, Conditions of Raman active Vibrations, Selection rules, Polarized and Depolarized Raman lines Study of: (Simple molecules such as SO_2, CO_2, N_2O and C_2H_2; (b) Hydrogen Bounding and (c) Metal ions in solution, Mutual exclusion principle, Problems related with Raman Spectra and its interpretation	
Unit IV	**Microwave spectroscopy:** Rotational Spectroscopy, Rotational spectra of diatomic	

	molecules based on rigid rotator approximation, Determination of bond lengths and/or atomic masses from microwave data, Effect of isotopic substitution, Non-rigid rotator, Classification of polyatomic molecules, Energy levels and spectra of symmetric top molecules and asymmetric top molecules and applications	
Recommended Books: 1. Spectroscopy by H. Kaur 2. Molecular Spectroscopy by Benwell 3. Spectroscopy by B.K. Sharma 4. Spectroscopy of organic Compounds by P.S. Kalsi 5. Vibrational Spectroscopy theory and applications by D.N. Sathyanarayana		
Paper II	**MCHT-102**	
Physical Chemistry (Chemical Kinetics and Classical Thermodynamics)		
Course Objectives: The objective of this course is to provide students a new and advance understanding of Transition state theory, Limitation of Lindemann theory, Hinshelwood treatment, RRK theory, salt effects, RRKM theory and advances made by Slater. It also gives knowledge of collision cross-section, Inter-molecular potential, potential energy surfaces, elastic molecular collisions, general features of fast reaction and their measurement technique. provide comprehensive and rigorous treatment of classical thermodynamics, thermodynamics relations. Explain the concept of partial molar properties fugacity and activity. It provides knowledge of entropy production, irreversible process and Onsager's reciprocity. **Course Outcome:** After successful completion of this course 1. Students will be able to understand the collision theory and theory of absolute reaction rates. Statistical treatment of unimolecular reaction including Lindemann theory, Hinshelwood treatment, RRK theory (salient features and limitations) RRKM theory and advances made by Slater. 2. Students will be able to understand fast reaction: Flow system, Relaxation methods, Flash photolysis 3. Students will acquire an ability to learn Collision cross-section, Inter- molecular potential, potential energy surfaces and elastic molecular collisions.		

4. Students will be able to understand various thermodynamic relationships, the concept of free energy and partial molar quantities, fugacity, activity and activity coefficients and determination, third law of thermodynamics 5. Students will be able to understand thermodynamic criteria in non-equilibrium state, entropy production and their applications.		
Unit I	**Theories of Reaction Rates:** Collision Theory of reaction rates, steric factor. Arrhenius equation and collision theory. Theory of absolute reaction rates. Thermodynamic formulation of reaction rates, comparison of Eyring equation and Arrhenius equations. Comparison of transition state theory and collision theory. Lindemann's mechanism of unimolecular gaseous reaction. Hinshelwood mechanism, RRK theory and RRKM theory, ionic reactions, salt effects (primary and secondary)	
Unit II	**Chemical dynamics:** Dynamic chain reaction, H_2-Br_2, decomposition of ethane and acetaldehyde. Photochemical combination of H_2-Br_2, and H_2-Cl_2 reactions. Oscillatory chemical reactions. Kinetics of enzyme reactions (Michaelis Menten Equation, Lineweaver-Burk Plot). General features of fast reactions, study of fast reactions; by flow method, relaxation method, flash photolysis and magnetic resonance method.	
Unit III	**Some Important Thermodynamic Relationships:** The Joule Thomson's effect, The Gibbs- Helmholtz equation and its application, The Clausius - Clapeyron equation, The Maxwell's relations. **Partial molar Properties:** Partial molar quantities, (partial molar volume and partial molar Gibbs energy), Chemical potential and variation of chemical potential with temperature and pressure, The Gibbs Duhem equation and its applications. **Fugacity and Activity:** Fugacity, variation of fugacity with temperature and pressure, Activity and the activity coefficient.	

Unit IV	**Third law Thermodynamics:** The third law, Nernst heat theorem, application of third law, The residual entropy. Thermodynamics of Irreversible Processes: Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces, non- equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation, non –linear thermodynamic treatment of electro- kinetic phenomena, thermo-osmosis and reverse osmosis.	
	Books Recommended: 1. K. J. Laidler, Chemical Kinetics, 3rd edition (1987), Harper & Row 2. I.N. Levine, Physical Chemistry, 5th Edition (2002), Tata McGraw Hill Pub. Co. Ltd., New Delhi. 3. Thermodynamics for Chemists by S. Glasstone. 4. An Introduction of Chemical Thermodynamics by R.P. Rastogi and R.R. Mishra. 5. Comprehensive Physical Chemistry by N.B. Singh, S.S. Das and N.S. Gajbhiye, New Age International Publishers. 6. P.W. Atkins, Physical Chemistry, Oxford University Press, New York.	
Paper III		**MCHT-103**
Inorganic Chemistry (Chemistry of Main Group Elements)		
Course Objectives: 1. Understand and apply stereochemical principles to predict the geometry of main group element compounds using VSEPR theory. 2. Analyze molecular shapes using Walsh diagrams and evaluate the factors affecting the stereochemistry of molecules and ions. 3. Explore the nature and implications of dπ–pπ bonding, Bent's rules, and hybridization energetics in main group compounds. 4. Investigate the synthesis, structure, bonding, and industrial relevance of polyether complexes, polyphosphazenes, thiazyl compounds, and tetrasulphur dinitride.		

5. Examine the structural and bonding features of boranes, carboranes, and related anionic species. 6. Study the synthesis, bonding, and structural diversity of carbides, polyanions, and silicates including their classification. **Course Outcome:** 1. Students will able to Apply VSEPR theory and steric principles to predict and explain the shapes of molecules and ions with 2–7 electron pairs in the valence shell. 2. Interpret and construct Walsh diagrams to rationalize geometry changes in triatomic and penta-atomic molecules. 3. Explain the formation and importance of dπ–pπ bonds and apply Bent's rule to rationalize hybridization patterns and molecular stability. 4. Describe the preparation methods, structural characteristics, and technical applications of polyether complexes, polyphosphazenes, thiazyl polymers, and S_4N_2 compounds. 5. Analyze the bonding and structural diversity in boranes, carboranes, and their anions using Wade's rules and molecular orbital theory. 6. Classify and describe the structures of silicates, and evaluate the synthesis and bonding in carbides and polyanions of heavier main group elements like Ge, Sn, Pb, Sb, Bi, and Hg.		
Unit I	**Stereochemistry of Bonding Among Main Group Elements:** VSEPR theory, stereochemical rules and explanation of shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs. Walsh diagram (tri- and penta-atomic molecules) dπ-pπ bonds, Bent's rules. Energetics of hybridization	
Unit II	**Compounds of Main Group Elements:** Preparation Structure Bonding and Technical application of Polyether complexes of alkali and alkaline earth metals; Polyphosphazenes and Thiazyl & its polymers, tetrasulphur dinitride.	
Unit III	**Structure and Bonding in ions of Some Main Group Elements:** Structure and bonding in borane anions, higher boranes, carboranes.	

Unit IV	**Carbides, Polyanions &Silicates:** Synthesis and structure of carbides & polyanions of Ge, Sn, Pb, Sb, Bi and Hg. Classification and structures of silicates.	
	Books Recommended: 1. Advanced inorganic Chemistry, 6th Edition F. A. Cotton and G. Wilkinson. 2. Principles of Structure and Reactivity 4th Edition J. E. Huheey, E. A. Keiter and R. L. Keiter 3. Chemistry of Elements N. N. Greenwood and A. Ernshaw 4. Organometallic Chemistry: A Unified Approach R. C. Mehrotra and A. K. Singh	
Paper IV		**MCHT-104**
Organic Chemistry (Organic Reaction Mechanism)		
Objective: Primary aim of this course is to develop interest and skill for generating mechanistic path for organic transformations in the students. The focus of this course is to give the detailed insight of organic reaction mechanism and to understand the physical chemistry of organic reactions along with the nucleophilic substitution reaction, elimination reaction & Addition on Carbon-Carbon double bond. **Outcome:** After completion of the course students will understand the mechanistic pathways of the various organic reactions. Students will become competent to predict the chemo-, regio- and stereoselective outcome of such reactions.		
Unit I	Determination of Organic Reaction Mechanism: Potential energy diagram, Transition states and intermediates, Hammond's Postulate, Methods of determination of organic reaction mechanism, Kinetic isotopic effect and its importance in the determination of reaction mechanism, The Hammett equation and linear free energy relationship, substituent and reaction constants	
Unit II	**Substitution Reaction:** Aliphatic Nucleophilic Substitution at Saturated Carbon Atom: Mechanism and stereochemistry of SN^1, SN^2, and SN^i reactions. Role of structure of substrate, nucleophile, leaving group and solvent on SN reactions, nucleophilic substitution in bridged systems, Neighbouring Group Participation:	

	Evidence for NGP, Participation by phenyl group, π and σ bonds, and Anchimeric Assistance.	
Unit III	**Elimination Reaction:** Mechanism and Stereochemistry of E1, E2 and E1cb elimination, factors affecting E1, E2 and E1cb reactions, orientation (Saytzeff and Hofmann Rule), Pyrolytic (syn) elimination (Chugaev and Hoffman elimination), Competition between substitution and elimination reactions, Peterson Elimination, Julia Olefination	
Unit IV	**Addition on Carbon-Carbon double bond:** Mechanism and Stereochemistry of addition of halogen (X2), Halogen acids (HX) to alkenes and its regioselectivity, 1,2-Bishydroxylation, Epoxidation, Hydroboration-Oxidation and Oxymercuration-Demercuration **Addition to Carbon-Oxygen double bond:** Aldol Condensation, Stobbe Condensation, Cannizaro Reaction, Benzoin condensation. **Addition on Conjugated Alkene:** Addition of halogens on butadiene, Michael Addition	

Recommended Books

1. Advance Organic Chemistry–Structure and Mechanism, J. March, John Wiley
2. Advanced Organic Chemistry-F. A. Carey and R. J. Sundberg A
3. Advanced Organic Chemistry-F. A. Carey and R. J. Sundberg B
4. Modern Methods of Organic Synthesis-W. Carruthers & I. Coldham
5. Modern Organic Synthesis-Zweifel & Nantz

Paper V	**MCHP-105**

Practicals

Physical Chemistry:

1. Determine the solubility of benzoic acid in water at different temperatures and calculate the heat of solution.
2. Determine the distribution coefficient of benzoic acid between benzene and water.
3. Determine the distribution coefficient of acetic acid between benzene and water.
4. Determine the distribution coefficient of iodine between carbon tetra chloride and water.

5. Study the adsorption of acetic acid on charcoal and draw the Freundlich isotherm.
6. Show that the order of reaction between acetone and iodine is zero with respect to iodine.

Inorganic Chemistry:

1. Qualitative analysis of an inorganic mixture of seven radicals including Tl, W, Se, Te, V, Be, U, Ti, Zr, Th, Ce and Li, in addition to the radicals prescribed for the B.Sc. Course. Semi micro analysis is to be done.
2. Chromatographic separation of metal ions given in any one of the following combinations:

(a) Pb^{2+}, Ag^{+}, Hg^{2+}
(a) Co^{2+}, Ni^{2+}, Cu^{2+}
(a) Fe^{3+}, Cr^{3+}, Al^{3+}
(a) Ba^{2+}, Sr^{2+}, Ca^{2+}

Organic Chemistry:

1. Analysis of primary binary organic mixture (liquid-liquid, liquid-solid, solid-solid).
2. Determination of equivalent weight of organic acids by direct titration method.

M.Sc. II Semester		
Paper I		**MCHT-201**
Analytical Chemistry		
Objective: To provide basic understanding of the principles, instrumentation and application of chemical analysis techniques. **Outcome:** On completion of the course, students acquire knowledge to select proper techniques and instrumentation for particular sample analysis.		
Unit I	**Electroanalytical Techniques:** (a)Conductometric: Discussion of the nature of the curves of acid-base (including mixtures of acids), precipitation and complexometric titrations. (b)Potentiometric: different types of electrodes, discussion of nature of the curves for oxidation-reduction and acid-base titrations, comparison with the conductometric method. (c)Voltammetry, Cyclic voltammetry (d)Polarography: Dropping mercury electrons and its advantages, polarographically active species, concept of residual, diffusion and limiting current of	

	half-wave potential, Ilkovic equation and factors affecting diffusion current.	
Unit II	Thermo-analytical Methods: (a)Thermo-gravimetry: apparatus, factors affecting TGA, interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$ (b)Differential Thermal Analysis: Apparatus, factors affecting DTA curves with Special reference to heating rate, Particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts of metal hydrates.	
Unit III	Radiochemical methods: (a) Isotope Method (b) Inverse Isotopic Dilution (c) Neutron activation technique.	
Unit IV	Chromatographic Method: (a) Gas Chromatography: GLC and GC (b) HPLC	

Recommended Books

1. Fundamentals of analytical chemistry, D.A. Skoog, D.M. West and F.J. Holler
2. Quantitative inorganic analysis, A.I. Vogel
3. Instrumental Methods of Chemical Analysis, B.K. Sharma
4. Instrumental Methods of Chemical Analysis, H. Kaur
5. Analytical Chemistry, Gary D. Christian

Paper II	**MCHT-202**
Physical Chemistry (Quantum Mechanics and Surface Chemistry)	

Course Objectives:

The objective of this course is to provide students a new and advance understanding into quantum mechanics and surface chemistry

Course Outcome:

1.After successful completion of the course, the student will be able to:

Solve basic quantum mechanical problems using Schrödinger equation (particle in a box, harmonic oscillator, rigid rotator and hydrogen atom

2.Interpret the principles of quantum chemistry in the context of atomic and molecular structure. 3.Interpret the approximate methods to solve the molecular problems 4.Describe the concepts of surface chemistry including adsorption and colloids. 5.Analyse adsorption isotherms and interpret experimental surface phenomena data.		
Unit I	**Basic principles of quantum mechanics:** Postulates; operator algebra; exactly- solvable systems: particle-in-a-box, harmonic oscillator, rigid rotator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunnelling.	
Unit II	**Approximate methods:** The variation theorem, linear variation principle. Perturbation theory (first order and nondegenerate). Simple application of variation method in perturbation theory. Many –Electron Atoms: Antisymmetry and Slater determinant for the wave function of ground state of multielectron atom, Self consistent field approximation (Hartree's Theory).	
Unit III	**Surface chemistry:** Adsorption Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation surface area (BET equation), and surface film of liquids (electro –kinetic phenomenon) catalytic activity at surface.	
Unit IV	**Micelles:** Surface active agent, classification of surface-active agent, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactant, counter ion binding to micelles, thermodynamics of micellization – phase separation and moss action models, solubilization, micro emulsion, reverse micelles.	
	Books Recommended: 1.Quantum Chemistry by Donald A. Macquarrie	

	2.Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman 3.Quantum Chemistry by R. K. Prasad 4.Introductory Quantum Chemistry by A. K. Chandra 5.Quantum Chemistry by Ira N. Levine 6.Advance Physical Chemistry (Vol-1,2,3,4), K.L. Kapoor, MacMillan, India 4. 7.Advance Physical Chemistry; Puri Sharma Pathania,	
Paper III		**MCHT-203**
Inorganic Chemistry (Chemistry of Transition Metals)		

Objective: The objective of this course is to

1. Understand the chemistry of transition metal-carbon multiple bonds with emphasis on metal carbenes and carbynes, including their synthesis, bonding, and structural aspects.

2. Examine the kinetics and mechanisms of ligand substitution reactions in coordination complexes, particularly in octahedral Co(III) and square planar Pt(II) systems.

3. Analyze stereoisomerism in six-coordinate octahedral complexes and understand stereochemical rearrangements and racemization mechanisms.

4. Explore the theories and principles governing metal-ligand equilibria in solution, including formation constants and their experimental determination.

5. Apply both qualitative and quantitative methods to evaluate the thermodynamic stability of metal complexes.

Course Outcome: Students will able to

1. Explain the structural and bonding characteristics of low-valent transition metal carbenes and carbynes, and outline their methods of synthesis.
2. Analyze the kinetics and mechanisms of ligand substitution reactions in Co(III) and Pt(II) complexes using associative and dissociative pathways.

	3. Identify and predict the number and types of stereoisomers in octahedral complexes, including those with mono-, bi-, and polydentate ligands. 4. Describe and distinguish between stereochemical rearrangement mechanisms such as Bailar and Ray–Dutta twists and explain racemization processes in tris(chelate) complexes. 5. Define stepwise and overall formation constants, and analyze the factors influencing complex stability based on the properties of metal ions and ligands. 6. Determine stability constants of metal-ligand complexes using pH-metric and spectroscopic methods and interpret the results in terms of coordination chemistry principles	
Unit I	**Compounds of Transition Metal-Carbon Multiple Bond:** Carbenes and Carbynes: Low valent carbenes and carbines, synthesis, nature of bond and Structural Characteristics.	
Unit II	**Kinetics and mechanism of substitution reactions** in octahedral Co (III) and square planar Pt (II) complexes.	
Unit III	**Stereoisomerisms** in six coordinate octahedral complexes (Ma_3bcd, Ma_2bcde, Mabcdef and complexes containing bi- and ter -dentate ligands, intermolecular and intramolecular rearrangements (Bailar and Ray-Dutt Twist) Mechanism of racemization in tris (chelate) octahedral complexes, methods of resolution of optical isomers.	
Unit IV	**Metal Ligand Equilibria in Solution:** Step wise and overall formation constants and their relations, Factors affecting the stability of metal complexes with reference to the nature of metal ions and ligands, determination of stability constants by pH-metric and spectroscopic methods.	
	Books Recommended: 1. Inorganic Chemistry, 4th Edition, Principles of Structure and Relativity by J.E. Huheey, E.A. Keiter and R.L. Keiter, 1993	

	2. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths, 1997 3. Mechanism of Inorganic Reactions; A Study of Metal Complexes in Solution by F. Bosolo and R.G. Pearson	
Paper IV		**MCHT-204**
Organic Chemistry (Stereochemistry and Pericyclic Reactions)		
Objective: This course is framed to provide an in depth understanding of some important aspects of Stereochemistry, pericyclic reactions, Stereochemistry and reactivity of cyclohexane and asymmetric synthesis. **Outcome:** On the completion of the course students will have the understanding of basics of organic Photochemistry and Pericyclic reactions. Various theories/rules governing these pericyclic reactions will help them to predict the products with stereochemistry involved in these reactions.		
Unit I	**Stereochemistry:** Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, Configurational projections (Wedge-dash, Fischer, Newmann and Saw-Horse projections), Interconversion of different projections, CIP rule and R/S nomenclature, **Principle of axial and planar chirality:** optical isomerism of biphenyl, allenes, spiranes, cyclophane, ANSA compounds optical activity due to intramolecular overcrowding, absolute configuration, **Topicity and Prostereoisomerism:** Introduction, Homotopic, enantiotopic and diastereotopic atoms, groups and faces, Nomenclature and symbols	
Unit II	**Asymmetric synthesis:** Racemic mixture, Enantiomeric excess and optical purity, stereoselectivity (enantioselectivity and diastereoselectivity) and stereospecificity, Diastereoselective aldol condensation with special emphasis on Cram's rule, Felkin-Anh Model and Zimmerman-Traxler Model **Asymmetric synthesis:** Principles of asymmetric synthesis, Asymmetric synthesis involving chiral auxiliary (Evans Auxiliary), chiral reagent and chiral	

	catalysis example: CBS reagent, Sharpless Asymmetric epoxidation,	
Unit III	**Stereochemistry and reactivity of cyclohexane and its derivatives:** Configuration, conformation and stability of mono and di-substituted cyclohexane and cyclohexanones, Stereoisomerism (cis-trans and chirality) of disubstituted cyclohexanes. Effect of conformation on Reactivity of substituted cyclohexane	
Unit IV	**Pericyclic reactions:** Introduction, classification and characteristics, Conservation of Molecular orbital symmetry, Use of correlation diagrams: FMO approach to study electrocyclic reactions of linear conjugated diene, triene and allyl systems., Cycloaddition reactions involving [2+2] and [4+2] systems., Sigmatropic rearrangements ([1,3], [1,5] and [3,3]), Claisen, Cope, and aza-Cope rearrangements, Wolff Rearrangement, Wittig Rearrangement, Group transfer reactions such as Conia-ene reaction	

Recommended Books

1. Pericyclic Reaction and Organic Photochemistry BY Dr. Vinay Prabha Sharma, Rakesh Kumar
2. Organic Synthesis BY Dr. Jagdamba Singh, Dr. L.O.S. Yadav
3. Stereochemistry By P. S. Kalsi
4. Stereochemistry by D Nasipuri

Paper V	**MCHP205**

Practicals

Physical Chemistry:

1. Draw the solubility curve for water-acetic acid- chloroform system.
2. Study the adsorption of oxalic acid on charcoal and draw the Freundlich isotherm.
3. Determine the rate constant of the acid-catalyzed hydrolysis of ethyl acetate at laboratory temperature.
4. Determine the rate of constant of the hydrolysis of ethyl acetate by sodium hydroxide at laboratory temperature.
5. Carry out the conductometric titration between the strong acid and strong alkali.

6. Determine the dimerization constant of benzoic acid in benzene medium by partition method.
7. Determine the solubility of salicylic acid in water at different temperatures and calculate the heat of solution.

Inorganic Chemistry:

Either both gravimetric and one volumetric estimation of two metal ions from following mixtures:

(a) Cu^{2+} and Ni^{2+}
(b) Cu^{2+} and Zn^{2+}
(c) Ni^{2+} and Zn^{2+}
(d) Cu^{2+} and Ba^{2+}
(e) Cu^{2+} and Ag^{+}
(f) Fe^{2+} and Ag^{+}
(g) Ba^{2+} and Ag^{+}

Organic Chemistry:

1. Preparation of organic compounds involving two stages, Emphasis should be given in the following Processes:
2. Purification, distillation under reduced pressure, steam distillation, and fractional crystallization

M.Sc. III Semester	
Paper I	**MCHT-301**
Select Topics in Chemistry	

Course Objectives:

By the end of this course, students will:

1.Understand the fundamental principles of molecular symmetry and apply group theory to chemical systems.

2.To introduce the principles of green chemistry, its importance, and sustainable methodologies such as atom economy, microwave/ultrasound-assisted synthesis, and catalysis.

3. Gain knowledge of the structure, classification, and interactions of biopolymers like proteins, nucleic acids, and polysaccharides.

4.To develop an understanding of the Hard and Soft Acids and Bases (HSAB) concept, its theoretical basis, applications, and use in molecular modelling.

Course Outcomes (COs)

After successful completion of this course, students will be able to:

1. Identify symmetry elements and apply group theory to classify molecules into point groups.

2. Apply the principles of green chemistry to design environmentally friendly chemical processes using modern techniques like biocatalysis and photochemistry. 3. Describe the structure, functions, and types of biopolymers and their biological importance. 4. Classify and predict reactivity using the HSAB principle and employ hardness/softness descriptors in molecular modelling.		
Unit I	**Symmetry and its applications:** Symmetry elements and symmetry operations with special reference to water, ammonia and ethane, Classification of molecules/ ions based on their symmetry properties, Derivation of matrices for rotation, reflection, rotation-reflection and inversion operations. Direct products, Symmetry point groups applied to all type of molecules (C_{nh}, D_{nh}, C_{nv}, T_d, O_h and I_h). Group multiplication basis, matrix representation, character of an operation, orthogonality, reducible and irreducible representations.	
Unit II	**Green Chemistry:** Introduction & importance of green chemistry, Limitations in the pursuit of the goals of Green Chemistry, Twelve principles of Green Chemistry, Prevention of Waste/ by-products, Atom Economy, use of microwaves and ultrasonic energy, bio catalysis and photo catalysis.	
Unit III	**Drug Design:** Drug discovery process–traditional approach and rational approach. Biological activities, definition, types and measurements, Introduction to Pharmacokinetics and Pharmacodynamics, ADMET properties, Concept of Drug Receptor interaction, Theories of drug receptor interaction: Occupancy theory, rate theory, induced fit theory, Introduction to Structure activity relationship (SAR) and Quantitative Structure activity relationship (QSAR), Bio-isosterism, Introduction to computer aided drug design, Concept of Pharmacophore.	
Unit IV	**Hard and Soft Acids and Bases (HSAB) Principle:** Classification of acids and bases as hard and soft, Theoretical basis of hardness and softness, Pearson's HSAB concept, Acid – Base strength, hardness and softness., Application and limitations of HSAB	

	principle. Hardness and Softness as Descriptors in Molecular Modelling.	

Recommended Books:

1. F. A. Cotton; Chemical Applications of Group Theory, 3rd edition, (1999), John Wiley &Sons, New York
2. K. Veera Reddy; Symmetry and Spectroscopy of Molecules; New Age International Pvt. Ltd., New Delhi (1999).
3. An Introduction to Medicinal Chemistry Seventh Edition, Graham L. Patrick, Publisher, Oxford University Press, 2023
4. The Organic Chemistry of Drug Design and Drug Action, Richard B. Silverman, Academic Press Inc.
5. Paul T. Anastas and John C. Warner, Green Chemistry: Theory and Practice

Paper II	**MCHT-302**
Physical Chemistry (Advanced Quantum Mechanics)	

Course Objectives

The course aims to:

1.Understand the fundamentals of quantum mechanics applied to molecular systems.
2.Gain insight into Hückel Molecular Orbital Theory and its applications in conjugated systems.
3.Comprehend the concepts behind Semi-Empirical and Ab Initio Self-Consistent Field (SCF) methods.
4.Develop an introductory understanding of Density Functional Theory (DFT) and its use in electronic structure calculations.
5.Learn the basic principles of Molecular Mechanics and its utility in modelling molecular systems.

Course Outcomes

After successful completion of the course, students will be able to:

1.Apply Hückel Molecular Orbital theory to analyse π-electron systems in conjugated molecules.
2.Compare and contrast Semi-Empirical and Ab Initio SCF methods for molecular structure prediction.
3.Demonstrate the ability to carry out basic quantum chemical calculations using *Ab-Initio* methods.
4.Explain the foundational principles of Density Functional Theory and its relevance to real-world systems.

5.Use Molecular Mechanics models to describe molecular geometry and predict structural parameters. 6.Evaluate the suitability of different computational approaches for a given chemical problem.		
Unit I	**Hückel Molecular Orbital Theory Of con jugated systems and its applications** Calculation of energy levels and delocalisation energy of butadiene, cyclic conjugated systems: cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, concept of aromaticity and antiaromaticity, Hückel treatment of linear polyenes.	
Unit II	**Semi- Empirical and Ab-Intio SCF Theories:** Semi- empirical SCF theory (CDNO, INDO & MNDO), Slater and Gaussian type orbitals, Configurational interaction and electron correlation, Moeller- Plasset Perturbation methods.	
Unit III	**Introduction to Density Functional Theory:** Concept of basis sets, The Hohenberg variational theorem and Kohn- Sham orbitals, The Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). Density Functional theory and its significance.	
Unit IV	**Introduction to Molecular Mechanics:** Force Fields, Energy Calculations, Different types of force fields and their comparison	
	Books Recommended: 1. Atkins, P. W. & Friedman, R. S. Molecular Quantum Mechanics 3rd Ed., Oxford University Press 2. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey 3. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings 4. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books	

Paper II	**MCHT-303**
Inorganic Chemistry (Coordination Chemistry)	

Course Objective: By the end of this course, students will able to 1. Apply Hund's rules, spin–orbit coupling, and inter-electronic repulsion parameters (Racah parameters) to determine ground and excited states of transition metal ions. 2. Analyze the effect of ligand fields on free ions using Orgel and Tanabe–Sugano diagrams, with focus on term mixing and correlation of energy levels in weak and strong fields. 3. Interpret the electronic spectra of transition metal complexes, including calculation of Dq, Racah B, and nephelauxetic β parameters, and understand Jahn–Teller effects. 4. Evaluate the magnetic properties of complexes based on spectroscopic terms, orbital contributions, and magnetic coupling phenomena. 5. Explore molecular orbital theory as applied to metal–ligand bonding in octahedral, tetrahedral, and square planar geometries, and understand the limitations of Crystal Field Theory (CFT). **Course Outcome:** Upon successful completion of this course, students will be able to: 1. Determine term symbols and energy terms for transition metal ions based on electronic configurations using Hund's rules, hole formalism, and angular momentum coupling. 2. Derive ground and excited term symbols for d^2 configuration and analyze spin–orbit coupling and inter-electron repulsion using Racah parameters B and C. 3. Construct and interpret Orgel and Tanabe–Sugano diagrams for d^2 ions, apply the non-crossing rule, and understand term mixing in ligand fields.	

4. Analyze the electronic spectra of octahedral complexes such as M(H_2O)_n^n+, apply selection rules, and compute crystal field splitting (Dq), B, and β parameters. 5. Identify and explain Jahn–Teller distortions and their influence on electronic spectra and geometry of complexes. 6. Assess the magnetic behavior (diamagnetism, paramagnetism, ferro-/antiferromagnetism) of complexes, including quenching of orbital angular momentum and term-based magnetic contributions.		
Unit I	**Energy levels in an atom:** Relation between electronic configuration and energy terms, coupling of angular angular momenta, coupling of spin angular momenta, spin-orbit coupling, energy terms. Determination of ground state term: Hund's rules. Determination of term symbol for a closed subshell. Hole formulation. Derivation of terms for d2 configuration. Inter electron repulsion parameter. Variation of Racah B and C parameters in different transition series. Spin orbit coupling parameters.	
Unit II	**Electronic Spectra of Complexes:** Splitting of electronic energy level and spectroscopic states, Orgel diagrams, mixing of terms, transition from weak to strong field, correlation diagram for only d^2 case, Non-crossing rule, Tanabe Sugano diagrams. Selection rules, Interpretation of the spectra of aqueous solution of $M[(H_2O)n]^{n+}$, Calculation of Dq, B and β parameters, Jahn-Teller distortion and its effect on electronic spectra.	
Unit III	**Magnetic Properties of Complexes:** Dia, para, ferro and antiferromagnetisms, Quenching of orbital angular momentum by ligand. The magnetic properties of A, E and T terms.	
Unit IV	**Metal-ligand Bonding:** Limitations of CFT, Nephelauxetic series, molecular orbital energy level diagram of octahedral, tetrahedral and square planner complexes.	
	Books recommended:	

	1. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and Its Applications, Willey, New York, 2000 2. D. Sutton, Electronics Spectra of Transition Metal Complexes. 3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules. 4. J. D. Lee , Concise Inorganic Chemistry Fifth Edition 5.Principles of Structure and Reactivity 4th Edition J. E. Huheey, E. A. Keiter and R. L. Keiter	
Paper II		**MCHT-304**
Organic Chemistry (Natural Products)		
Objective: The overall objective is to acquaint students with the fundamentals of natural products, Alkaloids, Terpenoids, Vitamins & hormones. **Outcome:** f this course, the student shall be able to: Get insights into plant derived therapeutic leads, Biogenesis of Natural Products, Terpenoids, and Alkaloids. Optimize the extraction technique according their chemical class. Perform a bioassay guided isolation to improve throughput for identification of potential bioactive natural products. Contribute towards the development of herbal formulations for the prophylactic use.		
Unit I	**Biogenesis of Natural Products:** The acetate hypothesis, isoprene rule, mevalonic acid from acetyl Co-enzyme A, Biogenesis of mono, sesqui, and diterpenes, Shikimic acid pathway for biogenesis of aromatic ring, General biosynthesis of alkaloids.	
Unit II	**Alkaloids:** Classification, General methods of structure elucidation of alkaloids, Structure and synthesis of–Nicotine, Morphine, and Coniine.	
Unit III	**Terpenoids:** Classification, Importance of terpenoids, Isoprene rule, Structural elucidation and synthesis of myrcene, α-terpinol and limonene	
Unit IV	**Steroids:** Basic Skeleton, Diels Hydrocarbon, Structural determination and synthesis of Cholesterol, Testosterone, Estrone and Progesterone	
Recommended Books 1. Organic Chemistry, Vol 2, I.L. Finar, ELBS 2. Natural Products by O P Agarwal		
Paper III		**MCHT-305**

<table>
<tr><td colspan="3">Physical Chemistry (Statistical Thermodynamics)</td></tr>
<tr><td colspan="2">Course Objectives
The course aims to:
1. Introduce the fundamental principles of classical and statistical mechanics.
2. Explain the derivation and significance of different statistical distributions (Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac).
3. Develop proficiency in calculating partition functions and connecting them to thermodynamic properties.
4. Apply statistical methods to interpret thermodynamic behaviors of gases, solids, and molecular systems.
Course Outcomes
After successful completion of the course, students will be able to:
1. Describe the foundational principles of classical statistical mechanics and microcanonical ensembles.
2. Derive and interpret molecular and canonical partition functions for simple systems.
3. Correlate partition functions with macroscopic thermodynamic properties like internal energy, entropy, and free energy.
4. Utilize statistical thermodynamics concepts in areas like chemical equilibrium, reaction</td><td></td></tr>
<tr><td>Unit I</td><td>Basics of Classical Statistical Mechanics: Fundamentals of statistical Mechanics, Phase space, Microstates, Macrostates, Ensemble (canonical, microcanonical and grand canonical), Ensembles-average, statistical weight factor, probability distribution, Liouville‟s theorem.
Distribution laws:
Energy levels, Boltzmann distribution law, Fermi–Dirac statistics and Bose–Einstein Statistics.</td><td></td></tr>
<tr><td>Unit II</td><td>Distributions & Thermodynamics:
The partition function, relation of the partition functions to the thermodynamic functions such as</td><td></td></tr>
</table>

	internal energy, heat capacity, enthalpy, free energy, entropy and chemical potential.	
Unit III	**Determination of Partition functions:** Localised and non–localised systems, Separation of the partition function, Translational partition function, The Sackur Tetrode equation, Rotational partition function, vibrational partition functions, electronic partition function, nuclear partition function Derivation of thermodynamic properties of ideal gases from partition functions.	
Unit IV	**Applications:** Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, Calculation of equilibrium constants of gaseous solutions in terms of partition function, Einstein theory and Debye theory of heat capacities of monatomic solids.	
	Books Recommended: 1. D. A. McQuarrie, Statistical Mechanics, Harper and Row Publishers, New York, 2. M. C. Gupta; Statistical Thermodynamics, New Age International, 2000. 3. Chandler; Introduction to Modern Statistical Mechanics, Oxford University Press. 4. Thomas Engel, Philip Reid; Physical Chemistry; Pearson Education, 3rdEdition. 5. Benjamin Widom; Statistical Thermodynamics: A Concise Introduction for Chemists, Cambridge University Press, 1st Edition, **2002**	

Paper III	**MCHT-306**
Inorganic Chemistry (Supramolecular Chemistry)	
Course Objective: By the end of this course, students will: 1. Understand the historical development and foundational concepts of supramolecular chemistry, including key Nobel Prize-winning contributions. 2. Identify and describe the various non-covalent interactions that govern supramolecular systems.	

3. Explain the concepts of chelate and macrocyclic effects and evaluate their significance and applications. 4. Explore the principles of molecular recognition, including static and dynamic types, and their roles in chemical and biological systems. 5. Analyze host design strategies, template effects (kinetic and thermodynamic), and self-assembly processes in supramolecular systems. 6. Understand host–guest chemistry through detailed study of macrocyclic hosts such as crown ethers, cryptands, and cyclodextrins. 7. Examine materials such as zeolites, clathrate hydrates, and other supramolecular architectures and their practical applications. 8. Investigate the interdisciplinary applications **Course Outcome:** Upon successful completion of this course, students will be able to: 1. Describe the origin and evolution of supramolecular chemistry, highlighting the contributions of Nobel laureates in this field. 2. Classify and explain different supramolecular interactions such as hydrogen bonding, π–π stacking, van der Waals forces, and electrostatic interactions. 3. Differentiate between chelate and macrocyclic effects and analyze their impact on stability and selectivity in host–guest systems. 4. Define molecular recognition and distinguish between static and dynamic recognition, including examples from biological systems (e.g., enzyme-substrate, antigen-antibody). 5. Evaluate the role of host design and the influence of template effects (kinetic vs. thermodynamic) on the construction of supramolecular architectures. 6. Discuss the principles and types of molecular self-assembly, provide biological examples (e.g., DNA	

helices, protein folding), and assess applications in nanotechnology and materials. 7. Illustrate the structures, syntheses, and functions of crown ethers, cryptands, and cyclodextrins, and assess their use in ion transport, drug delivery, and sensing. 8. Provide a brief overview of zeolites, clathrate hydrates, and their uses in catalysis, separation, and gas storage.		
Unit I	History, Definition, Noble prize winners of Supramolecular Chemistry. Different types of Supramolecular interactions, Discussion about Chelate and macrocyclic effects with their respective Applications.	
Unit II	Definition of molecular recognition, Static and dynamic molecular recognition, role of molecular recognition in biological systems. Discussion about host design in Supramolecular Chemistry, Template effect, Kinetic and Thermodynamic template effects and its applications. Discussion about molecular self-assemble giving its types, biological examples of molecular self-assembly and its applications	
Unit III	Definition of Host-Guest Chemistry, Give the structure, synthesis, properties and applications of following: (i) Crown ethers (ii) Cryptands (iii) Cyclodextrin	
Unit IV	Give Brief account of (i) Zeolites: properties and applications (ii) Clathrate hydrate and its applications (iii) Applications of Supramolecular Chemistry in various fields	
	Books Recommended: 1. Supramolecular Chemistry by JW Steel and JL Atwood 2. Principles and Methods in Supramolecular Chemistry by H Scheneider and A Yatsimirsky 3. Supramolecular Chemistry: An Introduction by F Vogtle.	

	4. Perspectives in Supramolecular Chemistry, Vol.2, Crystal Engineering and molecular recognition by Desiraju (Ed.)	
Paper III		**MCHT-307**
Organic Chemistry (Aromaticity, Rearrangements & Reagents)		
Objective: To foundational knowledge of the Aromaticity, Electrophilic and Nucleophilic Substitution, Rearrangements, Reagents. **Outcome:** After completing this course student will be able to understand the aromaticity and aromatic compounds, aromatic Electrophilic and Nucleophilic Substitution, Rearrangements, Reagents		
Unit I	**Aromaticity:** Concept of aromaticity, antiaromaticity, non-aromaticity and homo-aromaticity, Alternant and non-alternant systems, Aromaticity in Benzenoid, non-benzenoids (tropolone, azulene, annulenes, phenalene, ferrocene and fullerene) compounds, Hückel's rule, Craig's Rule, Möbius aromaticity	
Unit II	**Aromatic Electrophilic and Nucleophilic Substitution:** Aromatic Electrophilic Substitution: General view, energy profile diagram, Arenium ion mechanism (ArSE), ortho/ para ratio and ipso substitution. Aromatic Nucleophilic Substitution: Aromatic SN^1 and SN^2 reaction (ArSN). Addition –Elimination (ipso) and elimination- addition (benzyne) mechanisms, Effect of substrates structure, nucleophile and leaving group over rate of reaction, Select Examples: Sommelet–Hauser rearrangement, Van-Richter Rearrangement, Smiles Rearrangement	
Unit III	**Rearrangements:** Mechanism and application of Favorskii, Curtius, Schmidt, Demjanov, Lossen, Alkyne zipper reaction, Baeyer-Villager Rearrangement and Wagner–Meerwein rearrangement, Beckmann rearrangement	
Unit IV	**Reagents:** Preparation and application in organic synthesis of following: a) DCC, DDQ, CH_2N_2, LDA, R_2CuLi, and 1,3-dithane	

	b) Wilkinson's catalyst, Grubbs Catalyst, and Phase-transfer catalyst. c) Sulphur, and phosphorous ylides, enamines	

Recommended Books

1. Reaction Mechanism in Organic Chemistry -A.M. Mukherjee, S.P. Singh
2. Organic Chemistry Reaction and Reagents - O.P. Agarwal
3. Molecular Orbital Methods in Organic Chemistry (HMO) and PMO-William B. Smith
4. Name reactions and reagents in organic synthesis by Mundy, Ellerd & Favaloro-

Paper V	**MCHP-308**

Practicals

Physical Chemistry:

1. **pH-Metry:**
Determination of strength or concentration of strong acid and strong base, Determination of strength of weak acid by pH titration with a strong base, Verification of Henderson's equation.

2. **Conductometry:**
Equivalent conductance of strong electrolytes at infinite dilution, Conductometric titration of strong acid with strong base Conductometric titration of weak acid with strong base Titration of mixtures of acids Precipitation titration, Verification of Ostwald's dilution law Verification of Kohlrausch's Law

3. **Potentiometry**

Inorganic Chemistry:

1. Gravimetry estimation of three metal ions from following: Ag^{+}, Cu^{2+}, Ni^{2+}, Zn^{2+}, Fe^{3+}, Al^{3+}, Ba^{2+} and Mg^{2+}

2. EDTA Titration:
Estimation of Mg^{2+}, Zn^{2+}, and Mg^{2+} and Ca^{2+} in admixture.

3.Preparation and Characterization of some metal complexes.

Organic Chemistry

1. Multistep synthesis of organic compounds
2. Estimation of sulfur in organic compounds
3. Estimation of glycine

Paper VI	**MCHD-309**

Dissertation

M.Sc. IV Semester

Paper I	**MCHT-401**

Spectroscopy-II

Objectives: Principles and instrumentation of different molecular spectroscopic methods. • Qualitatively predict which signals are to be observed in the mass, NMR or ESR of Mossbauer Spectroscopy. **Outcomes:** On completion of the course, students should be able to combine, evaluate and interpret information from the various spectroscopic techniques in determination of molecular structure		
Unit I	**Mass Spectrometry:** Measurement technique (El, Cl, FD and FAB), Molecular base and molecular ions, various class of organic molecules, McLafferty rearrangement and retro-Diels-Alder Fragmentation, nitrogen rule and determination of molecular composition of organic compounds from mass spectral data	
Unit II	**Nuclear magnetic resonance: (A). ^{1}NMR:** The spinning nuclei, Chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, Chemical and magnetic equivalence, first and non-first order spectra, Simplification of complex spectra and NOE deuterium exchange, application in structural determination of simple organic. **(B). ^{13}CNMR:** General introduction, peak assignments, chemical shift, ^{13}C-^{1}H coupling, Off-resonance Decoupling, Deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR: COSY, and HETCOR, Application to simple organic	
Unit III	**Electron Spin Resonance Spectroscopy:** Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, Application to organic free radical, Methyl Free Radical, Naphthalene and Benzene free radicals	
Unit IV	**Mossbauer Spectroscopy:** Theory, Instrumentation, Applications-isomer shift, nuclear quadrupole coupling and hyperfine interaction, Problems related to Mossbauer Spectroscopy	
Recommended Books 1. Spectroscopy by H. Kaur		

2. Molecular Spectroscopy by Benwell 3. Spectroscopy by B.K. Sharma 4. Spectroscopy of organic Compounds by P.S. Kalsi 5. Vibrational Spectroscopy theory and applications by D.N. Sathyanarayana		
Paper II		**MCHT-402**
Physical Chemistry (Electrodics and Electrochemistry)		
Course Objectives 1.To provide a thorough understanding of ionic conductance in aqueous and non-aqueous media and its relevance in electrochemical systems. 2.To explain the theory and structure of the electrical double layer and its significance in electrode interfaces. 3.To introduce the principles of electrodics and kinetics of electrode processes. 4.To describe the mechanisms and prevention of corrosion and its industrial importance. **Course Outcomes** After successful completion of the course, students will be able to: 1.Analyse conductance behaviour in aqueous and non-aqueous media and correlate it with ionic mobility and solvation effects. 2.Interpret the structure and behaviour of electrical double layers and their influence on electrode kinetics. 3.Apply the principles of electrodics to understand electron transfer reactions at electrodes. 4.Evaluate different types of corrosion, their mechanisms, and methods of corrosion control. 5.Design and interpret simple electrochemical experiments and utilize electrochemical data for scientific and industrial applications.		
Unit I	**Conductance in aqueous and non-aqueous media** Debye Hückel and Onsager theory of strong electrolytes, Brief description of ion-association, Wein effect and Debye –Falkenhagen effect, Effect of ionic strength on the rate of ionic reactions. Ion dissociation, its effect on conductance, diffusion of electrolytes, measurements of diffusion coefficient, in relation to conductance	
Unit II	**Electrical Double Layer Theory**	

	The Helmholtz –Perin Theory, The Gouy- Chapman Theory, Stern Modification in the Gouy-Chapman Theory.	
Unit III	**Electrodics and Corrosion** The equilibrium exchange current density, Butler Volmer Equation, Tafel plot, high field and low field approximation, Electrodeposition and electropolymerization. The mechanism of corrosion of metals, corrosion current and corrosion potential, Electro- chemical corrosion theory, corrosion prevention.	
Unit IV	**Electrode Processes** Concentration polarization, deposition and decomposition potentials, Overvoltage, Limiting current density and Dropping Mercury Electrode.	
	Books Recommended: 1. J.O.M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 2 A & B, 2. Second Edition (1998), Plenum Press, New York. 3.Samuel Glasstone; An Introduction to Electrochemistry, East West Press. 4. P. H. Rieger; Electro Chemistry, 2nd Edition Chapman &Hall,1988. 5. D.R. Crow; Principles and Application of Electro Chemistry, Chapman and Hall,1988. 6. Thomas Engel, Philip Reid; Physical Chemistry; Pearson Education, 3rd Edition, 2001.	
Paper II		**MCHT-403**
Inorganic Chemistry (Organotransition Metal Chemistry)		
Course Objectives: By the end of this course, students will: 1. Understand the synthesis, bonding, structure, and reactivity of mono- and polynuclear metal carbonyl complexes using electron counting and molecular orbital approaches. 2. Explore the bonding nature in metal–CO and metal–NO systems, including structural types of bridging ligands and their spectral characteristics.		

3. Investigate the synthesis, structural features, and reactivity of π-complexes such as alkenes, alkynes, dienes, arenes, and their coordination to transition metals.
4. Apply the MO theory to understand bonding in metallocenes, particularly ferrocene and arene complexes.
5. Analyze key organometallic reaction mechanisms including oxidative addition, reductive elimination, insertion, β-hydride elimination, and ligand substitution.
6. Gain knowledge of important homogeneous catalytic cycles like hydrogenation, hydroformylation, polymerization, and industrial processes such as the Wacker and Fischer-Tropsch processes.
7. Understand the concept of fluxionality in organometallic compounds, and how NMR spectroscopy is used to study dynamic behavior in η^3-allyl and η^5-dienyl complexes

Course Outcomes

Upon successful completion of this course, students will be able to:

1. Describe the synthesis and structure of mono- and polynuclear metal carbonyls using Polyhedral Skeletal Electron Pair Theory (PSEPT) and electron counting methods.
2. Explain the nature of metal–CO and metal–NO bonding, and interpret IR (vibrational) spectra for structural elucidation of carbonyl and nitrosyl complexes.
3. Identify the bonding and structural features of transition metal π-complexes, including alkenes, alkynes, dienes, and arene ligands.
4. Apply molecular orbital (MO) theory to understand the electronic structure and stability of sandwich compounds such as ferrocene and arene complexes.
5. Illustrate and analyze the steps of key organometallic catalytic cycles, including ligand coordination/dissociation, oxidative addition, reductive elimination, and migratory insertion.

6. Describe and evaluate industrially relevant catalytic processes, including Wilkinson's hydrogenation, hydroformylation, Wacker process, Fischer-Tropsch synthesis, and olefin polymerization. **7.** Explain the concept of fluxionality in organometallic systems and analyze dynamic behavior in η^3-allyl and η^5-dienyl complexes using NMR spectroscopy.		
Unit I	**Metal Carbonyls:** Preparation, structure (Polyhedral Skeletal Electron Pair Approach) and reactions/properties of polynuclear metal carbonyls, Nature of M-CO bonding, principal reaction types, vertices of CO bridging: Metal nitrosyls: bonding and structure, Metal carbonyl-metal nitrosyl complexes, Carbonyl metal hydrides. Vibrational spectra of metal carbonyls for structure elucidation.	
Unit II	**Transition Metal π-Complexes:** Preparations, Important reactions relating on the ligands, Structural features and bonding of alkenes, alkynes, alkyls, diene, dienyl, arene complexes, MO approach of bonding in Ferrocene and arene complexes.	
Unit III	**Organometallic Catalyst:** General idea of important catalytic steps, ligands coordination, dissociation and elimination; nucleophilic attack on coordinated ligands & coordinated molecular oxygen. Oxidative addition, Reductive elimination and migration (insertion) β-Hydride elimination reactions. Homogenous Catalysis: Hydrogenation of alkenes using Wilkinson's catalyst, Hydroformylation of alkenes using Co and Rh catalysts, Wacker Process, Fischer-Tropsch Process, Polymerization of Olefins.	
Unit IV	**Fluxional Organometallic Compounds:** Study of Fluxionality and dynamic equilibria in compounds such as η^3- allyl and η^5 dienyl complexes with NMR spectroscopy.	
	Books Recommended:	

	1.Comprehensive Organometallic Chemistry, Ed. E.W. Abel, Abel, F.G.A. Stone and G. Wilkinson, Pergamon, 1982. 2. Advnaced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, `Wiley, 1999. 3. The chemistry of elements, N.N. Greenwood and A. Earnshaw, 1997. 4. Inorganic Chemistry, principles of structure and reactivity. J.E. Huheey, Harper, 1983. 5. Organometallic Chemistry (A unified approach), R.C. Mehrotra and A. Singh, Wiley Eastern, 1991	
Paper II		**MCHT-404**
Organic Chemistry (Stereochemistry and Pericyclic Reactions)		
Objective: This course aims to impart to the student, knowledge of: Protection and Deprotection of groups, Selective name reactions, Oxidation, Reduction mechanism and the importance of chirality in organic synthesis. Multi-component reactions as a tool for efficient atom economical reactions. **Outcome:** On completion of the course, the student should be able to: Understand the importance of organic synthesis and propose syntheses of molecules with control of the stereochemistry. Design chemical processes and products that eliminate the use or generation of hazardous substances		
Unit I	**Protection and Deprotection of groups:** Principles of protection and deprotection of alcohols, 1,2- and 1,3-diols, amines, carbonyls and carboxyl groups in organic synthesis.	
Unit II	**Selective name reactions and their application in organic synthesis:** Reformatsky Reaction, Robinson annulations, Shapiro, Hoffman-Loffter-Frytag reaction, Baylis-Hillman Reaction, Darzens Condensation, Wittig Reaction, Coupling Reactions (Suzuki Coupling and Sonogashira Coupling),	
Unit III	**Oxidation:** Mechanisms and application of: SeO_2, Jones reagent, Pyridinium chlorochromate (PCC), Corey-Kim Oxidation, Pfitzner–Moffatt oxidation, Swern Oxidation, Dess-Martin Oxidation, Davis Oxidation	
Unit III	**Reduction:** Birch reduction, Mechanism and stereochemistry of reduction of saturated/unsaturated carbonyl compounds with	

	following reagents: $NaBH_4$, LAH, DIBAL, diborane, and 9-BBN,	

Recommended Books

1. Pericyclic Reaction and Organic Photochemistry BY Dr. Vinay Prabha Sharma, Rakesh Kumar
2. Organic Synthesis BY Dr. Jagdamba Singh, Dr. L.O.S. Yadav
3. Stereochemistry By P. S. Kalsi
4. Stereochemistry by D Nasipuri

Paper III	**MCHT-405**
Physical Chemistry (Polymer Chemistry)	

Course Objectives:

1.To provide fundamental knowledge of polymers, their structures, properties, and classifications.
2.To impart an understanding of various polymerization techniques and their mechanisms.
3.To familiarize students with the methods of polymer characterization and degradation.
4.To introduce rheological behavior and mechanical properties of polymers.
5.To expose learners to the synthesis, properties, and applications of commercial polymers.

Course Outcomes

After successful completion of the course, students will be able to:

1.Understand and explain basic concepts, structures, and classifications of polymers.
2.Analyse and apply different polymerization techniques like addition, condensation, and co-polymerization.
3.Evaluate the thermal, chemical, and photodegradation behaviours of polymers.
4.Interpret the rheological properties and their relevance to processing and application of polymers.
5.Identify the structure–property relationships of specialty and commercial polymers and their applications.

Unit I	**Basic Concepts, Polymer Characterization and Polymerization:** General definition, Types and Classification of polymers, Concept of average molecular weights in	

	polymers: (Number average, Weight average, Viscosity average and Sedimentation average molecular weights), Concepts of Mono-dispersity, polydispersity, Significance of Molecular Weight, Distribution Curves of polymers. Kinetics and mechanism of condensation, Addition (Radical chain and Ionic chain), Coordination and Copolymerization	
Unit II	**Degradation of Polymers:** Types of degradation: Random degradation and Chain depolymerisation, A general idea of thermal, mechanical and oxidative degradation, Antioxidants and stabilizers.	
Unit III	**Rheology of Polymers:** Viscous flow (Newtonian and Non- Newtonian fluids), Rubber elasticity (thermodynamics of elasticity), Visco-elasticity, The glassy state and glass transition temperature.	
Unit IV	**Some Commercial and Speciality Polymers:** Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins silicone and PTFE polymers. Speciality polymers: Fire retarding polymers and electrically conducting polymers, liquid crystal polymer. Biomedical polymers – contact lens, dental, artificial heart, kidney, skin and blood cells – polymers.	
	Books Recommended: 1.F.W. Billmeyer, “Textbook of Polymer Science”, John Wiley &Sons, New York. 2.H.R. Allcock, F.W. Lampe and J.E Mark, “Contemporary Polymer Chemistry”, Pearson Education Prentice Hall, Singapore. 3.Charles E. Cariaher, “Polymer Chemistry: An Introduction”, Marcel Dekker Inc, New York. 4.U.R. Gowariker, N.V. Vishwanathan and J. Shreedhar, “Polymer Science”, New Age International Publishers, New Delhi.	

	5.S.S. Das and N.B. Singh, An Introduction to Polymer Science and Technology", New age International Publishers, New Delhi.	

Maa Pateswari University Balrampur

Paper III	**MCHT406**
Inorganic Chemistry (Bioinorganic Chemistry)	

Course Objectives

By the end of this course, students will:

1. Understand the role and mechanisms of metalloenzymes in biological systems, including enzymes involving Zn, Cu, Mo, and Co centers.
2. Study the structure, function, and oxygen-binding behavior of metalloproteins involved in dioxygen transport and storage.
3. Explore the biological and chemical mechanisms of nitrogen fixation, focusing on nitrogenase enzymes and synthetic model complexes.
4. Examine the biological processes involved in metal storage, transport, and biomineralization in organisms.
5. Analyze the role of metals in medicine, including both beneficial and toxic effects, metal deficiency-related diseases, and applications in diagnosis and therapy

Course Outcomes

Upon successful completion of this course, students will be able to:

1. Describe the structure and catalytic function of zinc enzymes such as **carboxypeptidase** and **carbonic anhydrase**, and explain their biological significance.
2. Explain the role of **copper enzymes** like **superoxide dismutase** in oxidative stress defense mechanisms.
3. Discuss the structure and function of **molybdenum-containing enzymes** such as **xanthine oxidase**, and describe the biological activity of **coenzyme B_{12}** (a cobalt complex).
4. Compare the structures and oxygen-binding behavior of heme and non-heme oxygen transport/storage proteins like **hemoglobin**, **myoglobin**, **hemocyanin**, and **hemerythrin**.
5. Evaluate synthetic model complexes of iron that mimic the function of dioxygen carriers.

6. Explain the process of **biological nitrogen fixation**, with focus on **molybdenum nitrogenase**, its structure, mechanism, and synthetic analogs. 7. Describe the structure and role of **ferritin**, **transferrin**, and **siderophores** in metal storage, transport, and iron homeostasis. 8. Analyze the significance of **metal ions in medicine**, identifying disorders caused by metal imbalances, and discuss the role of metals in **diagnostic imaging** and **anticancer therapies** (e.g., **cisplatin**).		
Unit I	**Metalloenzymes :** Zinc enzymes - carboxypeptidase, carbonic anhydrase; Copper enzymes - superoxide dismutase; Mobybdenum - xanthine oxidase; Coenzyme vitamin B12 .	
Unit II	**Transport and Storage of Dioxygen:**Heme proteins and oxygen uptake, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron.	
Unit III	**Nitrogenase:** Biological nitrogen fixation, molybdenum nitrogenase, other nitrogenase model systems.	
Unit IV	**Metal Storage, Transport and Biomineralization :** Ferritin, transferrin and siderophores; Metals in Medicine: Metal deficiency and diseases, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.	
	Books Recommended: 1. Bioinorganic Chemistry. R. N. Hay. Wiley. 1984. 2. The Inorganic Chemistry of Biological Processes. M. M. Hughes. Wiley 1981. 3. An Introduction to bioinorganic Chemistry. El Ichiro ochai. Allyn. 1977. 4. Inorganic Chemistry : Principles of structure and reactivity. J.E. Huheey Harper. 1983. 5. Advanced inorganic Chemistry. F.A. Cotton and G. Wilkinson. Wiley. 1999.	

Paper III	**MCHT-407**

Organic Chemistry (Select Topics In Organic Chemistry)

Objective: This course aims to impart to the student, knowledge of: Synthesis, properties and reactions of 3-, 4-, 5-, 6-, 7- and 8-membered heterocyclic compounds. applications of Retro-Synthesis, to study the Carbohydrates and Synthetic Drugs.

Outcome: On completion of the course, students should be able to: Rationalize the synthesis, structure and applications of organometallic compounds for organic transformations. Design the synthesis of industrially important compounds.

Unit 1	1. Heterocycles a. General introduction and nomenclature b. Chemistry of (i) Five membered: Pyrazole and imidazole, oxadiazole and thiadiazole and thiazole (ii) Six membered: Pyrazine, pyrimidine and pyridiazine	
Unit 2	2.Retro-Synthesis: Introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions. One group C-X and two groups C-X disconnection, Chemo selectivity.	
Unit 3	3.Carbohydrates: Structure elucidation of Disaccharides: Lactose, maltose, sucrose Structure, function and configuration of Polysaccharides: Cellulose, Starch and Glycogens	
Unit 4	Synthetic Drugs: A general study of important synthetic drugs of the following types: Sulpha drugs: Sulphanilamide derivatives, sulphathiazole, sulphathalidine, sulphasuccidine, sulphaguanidine, sulphadiazine. Antimalarials: 4-Aminoquinoline derivatives, chloroquine, santoquine, camaquin, 8- aminoquinoline. Anti-cancer agents: Nitrogen mustards, antimetabolites in cancer chemotherapy. Antitubercular agents: PAS, Thiosemicarbazones, hydrazides and thiocarbanilides	

Recommended Books

1. Heterocyclic Chemistry by Bansal, Raj K

2. Fundamentals of Heterocyclic Chemistry Importance in Nature and In the Synthesis Of Pharmaceuticals by Louis D Quin
3. Principles of Pharmaceutical Organic Chemistry 2/E by Nadendla
4. Organic Chemistry by Subrata Sengupta

Paper V	**MCHP-408**

Practicals

Physical Chemistry :

1.Chemical Kinetics:

1.1 Determination of rate constant of acid Hydrolysis of ester

1.2 Relative Strength of strong acids by studying the kinetics of hydrolysis of ester

1.3 Kinetics of reactions between Potassium Persulphate and Potassium iodide.

1.4 Kinetics of iodination of acetone

2. Optical Methods:

2.1 Colorimetry: Verification of Lambert's Beer Law

2.2 Refractometry

2.3 Spectroscopic methods of analysis: UV-Visible, IR

2.4 Polarimetry

Inorganic Chemistry :

Any two of the following exercises:

1. Potentiometry:

a. Acid-Base, Redox Titrations.

b. Determination of stability constants of suitable complex systems.

2. Conductometry

Acid-Base and precipitation Titrations

3. Colorimetry and Spectrophotometry:

Estimation of the following metals in solution V, Cr, Mo, Fe and Ni.

4. Flame Photometry:

a. Estimation of sodium and potassium in admixture.

b. Estimation of magnesium and calcium in tap water.

c. Estimation of calcium in calcium salt solution.

Organic Chemistry :

1.Analysis of ternary organic mixture

2. Estimation of glucose

3. Project work

Paper VI	**MCHD-409**

Dissertation