Course Structure and Detailed Syllabi of

Master of Science (M.Sc.)

in

CHEMISTRY

Department of Chemistry
JAGANNATH BAROOAH UNIVERSITY
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Introduction:

This document presents the detailed syllabus for the two-year Master of Science (M.Sc.) program in Chemistry at Jagannath Barooah University, Jorhat. The primary objective of this syllabus is to provide students with an advanced and in-depth understanding of fundamental chemical principles across all major disciplines – Inorganic, Organic, Physical, and Analytical Chemistry. Beyond core knowledge, it emphasizes exposure to cutting-edge research areas, modern analytical techniques, and interdisciplinary fields such as Green Chemistry, Nanomaterials, Computational Chemistry, and Medicinal Chemistry.

Designed under a Choice Based Credit System (CBCS), this syllabus offers flexibility through a selection of elective courses, allowing students to tailor their learning path according to their specific interests and career aspirations. It maintains a strong balance between theoretical instruction and extensive practical laboratory training, crucial for developing essential hands-on skills and a scientific temperament.

Through this thoughtfully structured curriculum, Jagannath Barooah University aims to equip its M.Sc. Chemistry graduates with critical thinking abilities, strong research aptitude, and the professional competencies necessary to excel in diverse roles within academia, research institutions, chemical industries, and related sectors, or to pursue further doctoral studies.

The curriculum encompasses Core Courses, Elective Courses (Discipline Specific Elective - DSE, Generic Elective (GE), and Ability Enhancement Courses (AEC). Evaluation will follow a Continuous Comprehensive Evaluation system.

Program Objectives and Outcomes

The program aims to impart key knowledge and expertise in chemical sciences, prepare students for careers in chemistry, and encourage further research and entrepreneurship.

Graduate Attributes:

- Communicate scientific work effectively in oral, written, and ICT formats.
- Understand chemistry's role in addressing social, economic, and environmental problems.
- Act with integrity and ethics in their profession.
- Analyze and identify entrepreneurship opportunities.

Program Outcomes (PO):

- Firm foundation in fundamentals and applications of current chemical and basic science (Physical, Organic, Inorganic, Analytical, Chemistry of life).
- Awareness of major issues in chemical research and competence in initiating, developing, and pursuing scientific research.
- Ability to seek new knowledge, skills, and manage relevant information.
- Training to work effectively and safely in the laboratory, both independently and in teams.
- Ability to design and carry out scientific experiments and draw logical inferences.

Note: The specific distribution of credits and marks for internal assessment and end-semester examinations will follow the guidelines of Jagannath Barooah University, in adherence to UGC norms. The detailed breakdown within units may be further adjusted by the Department of Chemistry at Jagannath Barooah University based on evolving academic requirements and faculty expertise.

Course Structure: Semester-Wise Distribution

The program is structured across four semesters, with a mix of Core, Elective, ability enhancement and Laboratory courses.

Credit-wise Course Framework

Semester	**Core**	**DSE**	**GE**	**AEC**	**Total Credit**
Semester I	4+4+4+2+2+2		4		22
Semester II	4+4+4+2+2+2		4		22
Semester III	4+4+4+2+2+2	2*		2	22
Semester IV	4	(4+4)*+4**		2	18
Total Credit	**58**	**14**	**8**	**4**	**84**

DSE: Discipline Specific Elective; GE: General Elective; AEC: Ability Enhancement Course

*Students have to opt for GE paper from another Department in Semester 1 & 2.

Semester-wise distribution of paper

SEMESTER I					
Course	**Paper Title**	**Course Title**	**Marks (End Sem + IA)**	**Credit**	**Marks**
Core 101	PCHMC-101	Inorganic Chemistry-I	100 (60+40)	4	100
Core 102	PCHMC-102	Organic Chemistry-I	100 (60+40)	4	100
Core 103	PCHMC-103	Physical Chemistry-I	100 (60+40)	4	100
Core 104	PCHMC-104	Chemistry Laboratory -I	50 (30+20)	2	50
Core 105	PCHMC-105	Chemistry Laboratory -II	50 (30+20)	2	50
Core 106	PCHMC-106	Chemistry Laboratory -III	50 (30+20)	2	50
GE 107	PCHMG-207	Green and Sustainable Chemistry	100 (60+40)	4	100
Total			**550**	**22**	**550**
SEMESTER II					
Course	**Paper Title**	**Course Title**	**Marks (End Sem + IA)**	**Credit**	**Marks**
Core 201	PCHMC-201	Inorganic Chemistry-II	100 (60+40)	4	100
Core 202	PCHMC-202	Organic Chemistry-II	100 (60+40)	4	100
Core 203	PCHMC-203	Physical Chemistry-II	100 (60+40)	4	100
Core 204	PCHMC-204	Chemistry Laboratory -IV	50 (30+20)	2	50
Core 205	PCHMC-205	Chemistry Laboratory -V	50 (30+20)	2	50
Core 206	PCHMC-206	Chemistry Laboratory -VI	50 (30+20)	2	50
GE 207	PCHMG-207	Materials Chemistry	100 (60+40)	4	100

Total			**550**	**22**	**550**
SEMESTER III					
Course	**Paper Title**	**Course Title**	**Marks (End Sem + IA)**	**Credit**	**Marks**
Core 301	PCHMC-301	Inorganic Chemistry-III	100 (60+40)	4	100
Core 302	PCHMC-302	Organic Chemistry-III	100 (60+40)	4	100
Core 303	PCHMC-303	Physical Chemistry-III	100 (60+40)	4	100
Core 304	PCHMC-304	Chemistry Laboratory -VII	50 (30+20)	2	50
Core 305	PCHMC-305	Chemistry Laboratory - VIII	50 (30+20)	2	50
Core 306	PCHMC-306	Chemistry Laboratory -IX	50 (30+20)	2	50
DSE 307	PCHMD-307	PROJECT-I	50 (30+20)	2	50
AEC 308	PCHMA-308	Analytical Chemistry-I	50 (30+20)	2	50
Total			**550**	**22**	**550**
SEMESTER IV					
Course	**Paper Title**	**Course Title**	**Marks (End Sem + IA)**	**Credit**	**Marks**
Core 401	PCHMC-401	General Approaches to Research	100 (60+40)	4	100
		Special Paper I (Any One)	100 (60+40)	4	100
DSE 402 DSE 404 DSE 406	PCHMD-402 PCHMD-404 PCHMD-406	Inorganic Chemistry-IV Organic Chemistry-IV Physical Chemistry-IV			
		Special Paper II (Any One)	100 (60+40)	4	100
DSE 403 DSE 405 DSE 407	PCHMD-403 PCHMD-405 PCHMD-407	Inorganic Chemistry-IV Organic Chemistry-IV Physical Chemistry-IV			
DSE 408	PCHMD-408	Project-II	100 (60+40)	4	100
AEC 409	PCHMA-402	Analytical Chemistry-II	50 (30+20)	2	50
Total			**450**	**18**	**450**

PCHMC: PG Chemistry Core Course; PCHMD: PG Chemistry DSE Course;

PCHMG: PG Chemistry GE Course; PCHMA: PG Chemistry AEC Course.

Total Credits: 84

Total Marks: 2100

Semester I

Detailed Syllabus - Semester I:

Core Course 101: **L3 T1 P0 C4**

Title of the Paper: Inorganic Chemistry-I

Paper Code: PCHMC-101

Credit: 04

Objectives: Basic knowledge of structures and bonding, acid-base concepts, and a broad foundation in inorganic biochemistry.

Expected Learner Outcome: Understand structural and bonding nature, acid-base chemistry, and the role of metals/non-metals in biological systems.

Unit I: Chemical Bonding (15 Lectures, 20 Marks)

- VSEPR Theory: Structure of molecules with lone pairs, hybridization, Bent's rule.
- LCAO-MO methods for diatomic (homo/heteronuclear) and tri/tetraatomic molecules.
- Bonding in electron-deficient compounds (boranes, carboranes, S-N, Se-N, P-N).
- Metallic and Metal-ligand bonding: Spinel, Perovskite, Crystal Field Theory, Transition metal MO and ligand field theory, ML_6 and ML_4 structures. Chemical periodicity, hardness, electronegativity.

Unit II: Acid Base and Redox Chemistry (10 Lectures, 15 Marks)

- Acid-Base concepts, strengths, non-aqueous solvents, superacids, Hard and Soft Acids and Bases (SHAB principle).
- Half-cell reactions, reduction potential, electrochemical series, corrosion, Nernst equation, Latimer and Frost diagrams, disproportionation, cyclic voltammetry.

Unit III: Bioinorganic Chemistry (20 Lectures, 25 Marks)

- Fundamentals, essential/non-essential elements, role of 3d block elements and non-metals in bio-systems.
- Oxygen carriers (Hemoglobin, myoglobin, hemerythrin, hemocyanin), Electron transfer proteins (Cytochromes, Iron-Sulphur), Nitrogen fixation.
- Metalloenzymes, corrinoids (B_{12}), carboxypeptidases, chlorophyll, photosynthesis, Na-K pump, crown ethers, organo-transition metal complexes in bioinorganic chemistry.

Text Books: K. Hussain Reddy (Bioinorganic Chemistry), Gary L. Miessler & Donald A. Tarr (Inorganic Chemistry).

Recommended Books: M.N. Hughes (The Inorganic Chemistry of Biological Processes), D.E. Fenton (Bio-coordination Chemistry), C.E. Housecraft & A.G. Sharpe (Inorganic Chemistry).

Core Course 102: **L3 T1 P0 C4**

Title of the Paper: Organic Chemistry-I

Paper Code: PCHMC-102

Credit: 04

Objectives: Fundamental knowledge on structure, reactivity, reaction mechanisms, disconnection approach, and spectroscopic techniques.

Expected Learner Outcome: Understand bonding, reactivity, properties, design synthetic methodologies, and characterize products using spectroscopy.

Unit I: Structure, Bonding and Reactivity (8 Lectures, 12 Marks)

- Aromaticity, antiaromaticity, homoaromaticity, metallocenes, tropolones, azulenes.
- Supramolecular chemistry: weak bonds, charge transfer complexes, inclusion complexes, crown ethers, cryptands, rotaxanes.
- Fullerenes, Graphenes, Phase transfer catalyst, Hammet equation, Taft equation, influence of reaction medium.

Unit II: Organic Reaction Mechanism (10 Lectures, 13 Marks)

- Transition state vs. reaction intermediate, energy profile, rate limiting step, catalysed/uncatalysed reactions, kinetic vs. thermodynamic control.
- Kinetic and non-kinetic methods (Isotope labeling, kinetic isotope effects, cross-over experiment), Reactivity-selectivity principle (chemoselectivity, regioselectivity, stereoselectivity, stereospecificity).
- Neighbouring group effects, generation, stability, and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes, nitrenes.

Unit III: Stereochemistry I (10 Lectures, 12 Marks)

- Prostereoisomerism, prochirality, homotopic/heterotopic ligands/faces, optical purity, enantiomeric excess.
- Chirality in allenes, spirans, biphenyls.
- Stereoselective synthesis (diastereoselective, enantioselective), Stereo-differentiating approach, Nucleophilic addition to aldehydes/ketones (Cram, Felkin-Ahn).
- Enantioselective synthesis (chiral reagent, catalyst, auxillary), Resolution (optical, kinetic).

Unit IV: Disconnection Approach in Organic Synthesis (7 Lectures, 10 Marks)

- Acceptor/donor synthons, umpolung, retrosynthesis of alcohols (Grignard, hydride transfer) and carbonyl compounds.
- One/two group C-X disconnections, one/two group C-C disconnections.
- Retrosynthesis of 1,2-, 1,3-, 1,4-, 1,5-, 1,6- difunctional compounds (O,O and N,O).
- Protecting groups (hydroxyl, dihydroxy, carbonyl, carboxyl, amino).

Unit V: NMR & IR Spectroscopy (10 Lectures, 13 Marks)

- NMR: Chemical shift, factors affecting chemical shift, spin-spin interaction, coupling constant, relaxation, NOE, double resonance, tickling.
- Proton and ^{13}C NMR of simple organic molecules, MRI, 2D NMR (NOESY, DEPT, INEPT), Instrumentation, FT NMR.
- IR: Application in organic spectroscopy.

Text Books: I. L. Finar (Organic Chemistry), P.S. Kalsi (Stereochemistry and Mechanism), Donald L. Pavia (Introduction to Spectroscopy), Peter Sykes (A Guidebook to Mechanism in Organic Chemistry).

Recommended Books: R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee (Organic Chemistry), Paula Yurkanis Bruice (Organic Chemistry), Jerry March (Advanced Organic Chemistry), D. Nasipuri (Stereochemistry of Organic Compounds), Earnest E. Eliel (Stereochemistry of Carbon Compounds), Subrata Sengupta (Stereochemistry of Carbon Compounds), S. Warren (Disconnection Approach in Organic Synthesis, Designing Organic Synthesis), Christine Willis and Martin Willis (Organic Reaction Mechanism), E.J. Corey and Xue Min Chen (The Logic of Organic Synthesis).

L3 T1 P0 C4

Core Course 103:

Title of the Paper: Physical Chemistry-I

Paper Code: PCHMC-103

Credit: 04

Objectives: Concepts of fugacity, activity, partial molar quantities, third law of thermodynamics, fundamentals of quantum mechanics, and basics of spectroscopy.
Expected Learner Outcome: Solve problems in thermodynamics, understand quantum mechanical viewpoint, basic principles of quantum chemistry, and apply spectroscopic knowledge.

Unit I: Equilibrium Thermodynamics (13 Lectures, 15 Marks)

- Fugacity, ideal/non-ideal solutions, activity and activity coefficient, excess functions.
- Partial molar quantities (chemical potential, partial molar volume), thermodynamics of mixing.
- Third law of thermodynamics, experimental verification, absolute entropy determination.

Unit II: Quantum Chemistry-I (12 Lectures, 15 Marks)

- Review of Quantum Mechanics: Postulates, operators, commutation relation, theorems.
- Model Systems: Free particle, particle in a box (1D, 3D), degeneracy.
- Simple Harmonic Oscillator, two-particle rigid rotor, particle in a ring, quantum mechanical tunneling.

Unit III: Spectroscopy (20 Lectures, 30 Marks)

- Electromagnetic spectrum, interaction with matter, natural line width, broadening, intensity, selection rules.
- Rotational (microwave) spectroscopy: Classification of molecules, rotational energy levels (HCl), selection rules, intensity, Stark effect, spectra of symmetric/asymmetric top molecules.
- Vibrational spectroscopy: Fundamental frequencies, selection rules, harmonic/anharmonic oscillators, vibration-rotational spectra, P, Q, R branches, hot bands, group frequencies, normal modes, symmetry.
- Quantum theory of Raman effect, selection rules, mutual exclusion principle, vibration-rotation Raman spectra, intensity.
- Electronic spectroscopy: Electronic transitions, selection rules, Frank-Condon principle, electronic spectra of polyatomic molecules, Fluorescence, phosphorescence, solvent effects, absorption/intensity shifts, Woodward-Fieser Rules.

Text Books: P.W. Atkins (Physical Chemistry), Ira N. Levine (Quantum Chemistry), C.N. Banwell and E.M. McCash (Fundamentals of Molecular Spectroscopy).

Recommended Books: I. N. Levine (Physical Chemistry), S. Glasstone (Thermodynamics for Chemist), A.K. Chandra (Introduction to Quantum Chemistry), P.W. Atkins & R.S. Friedman (Molecular Quantum Mechanics), D.A. McQuarrie (Quantum Chemistry), G.M. Barrow (Introduction to Molecular Spectroscopy).

L0 T0 P2 C2

Core Course 104:

Title of the Paper: Chemistry Laboratory-I

Paper Code: PCHMC-104

Credit: 02

Inorganic Lab I (Marks 30):

Preparation and characterization (conductivity, IR, UV-Vis) of complexes:

Potassium chromioxalate, Reinecke's salt, Tris-(thiourea) copper(I) sulphate, Potassium chromithiocyanate, Chloropentamine Cobalt(III) chloride, Nitropentamine Cobalt(III) chloride, Sodium ferrioxalate, Tetraammine Cu(II) sulphate, Hexa-amine Ni(II) chloride, Sodium Cobaltinitrite, NitritoPentamineCobalt(III) chloride, Hexamine Co(III) sulphate pentahydrate.

Core Course 105: **L0 T0 P2 C2**

Title of the Paper: Chemistry Laboratory-II

Paper Code: PCHMC-105

Credit: 02

Organic Lab I (Marks 30):

- Organic Estimation (glucose, sucrose, acetone, hydroxyl/amino groups)
- Separation and identification of organic compounds by TLC
- Preparation of green solvent (ionic liquid, DES).

Core Course 106 **L0 T0 P2 C2**

Title of the Paper: Chemistry Laboratory-III

Paper Code: PCHMC-106

Credit: 02

Physical Lab I (Marks 30):

- Kinetics experiments: Rate constant and activation energy of hydrolysis of methyl acetate (acid-catalyzed); velocity constant of ethyl acetate hydrolysis by NaOH; inversion of cane sugar; kinetics of iodine and acetone reaction; rate constant and order of $K_2S_2O_8$ and KI reaction (influence of ionic strength).

- Determine molar mass of polymer by viscometric method.
- Study of complex formation between Cu2+ and ammonia by distribution method.
- Determine radius of glycerol by viscosity.
- Determine partial molar volume of ethanol.

L3 T0 P1 C3

Generic Elective Course 107

Title of the Paper: Green and Sustainable Chemistry

Paper Code: PCHMG-107

Credit: 04

Objectives: Understand principles of green chemistry and its application for sustainable development.
Expected Learner Outcome: Knowledge of green chemistry principles, sustainable practices, and their application in chemical processes.

Unit I: Principles of Green Chemistry (15 Lectures, 18 Marks)

- Twelve principles of green chemistry, atom economy, E-factor, reaction mass efficiency.
- Life cycle assessment, toxicology, environmental impact.

Unit II: Green Solvents and Catalysis (15 Lectures, 17 Marks)

- Alternative solvents: Ionic liquids, supercritical fluids, water as a solvent, solvent-free reactions.
- Green catalysis: Heterogeneous catalysis, biocatalysis, photocatalysis, phase transfer catalysis.

Unit III: Green Synthesis and Industrial Applications (15 Lectures, 25 Marks)

- Green synthetic methodologies: Microwave-assisted, ultrasound-assisted, sonochemistry, solid-state reactions.
- Green chemical processes in industry: Pharmaceuticals, polymers, fine chemicals.
- Biomass utilization, renewable energy, waste minimization.

Text Books: P.T. Anastas & J.K. Warner (Green Chemistry: Theory and Practice), R. Luque, J. Campelo and J.M. Clark (Handbook of Green Chemistry).
Recommended Books: M. Lancaster (Green Chemistry: An Introductory Text), J. Clark and D. Macquarrie (Handbook of Green Chemistry and Technology).

Semester II

Detailed Syllabus - Semester II:

L3 T1 P0 C4

Core Course 201:

Title of the Paper: Inorganic Chemistry-II

Paper Code: PCHMC-201

Credit: 04

Objectives: Overview of inorganic reaction mechanism and application of group theory.

Expected Learner Outcome: Thorough concept of kinetics of inorganic reactions and importance of group theory in chemical science.

Unit I: Inorganic Reaction Mechanism (13 Lectures, 20 Marks)

- Lability and inertness, stability constants, chelate effect, thermodynamic and kinetic stability. Factors affecting stability, determination of stability constant (Jobs, Bjerrum's methods).
- Mechanism of ligand replacement reactions: Substitution in octahedral [Cr(III), Co(III)] and square planar [Rh(I), Pt(II), Pd(II)] complexes.
- Rate of water replacement, solvolysis, hydrolysis (acid/base), factors affecting substitution rate, trans effect (theories, importance), electron transfer reactions (inner/outer sphere).

Unit II: Symmetry and Group Theory (20 Lectures, 25 Marks)

- Matrices and matrix representation of symmetry operations, definition of group (finite, infinite), examples.
- Symmetry elements as elements of group, Point groups.
- Orthogonality theorem, reducible and irreducible representations, construction of character tables (C_{2v}, C_{3v}).
- Direct product representation. Projection operator, symmetry adapted linear combination (SALC) for C_{2v}, C_{3v}, D_{4h}, T_d point group molecules.

Unit-III: Chemical Application of Group Theory (12 Lectures, 15 Marks)

- Construction of hybrid orbitals (d^2sp^3, sp^3), IR absorption and Raman scattering spectroscopy (vibrational modes as bases, symmetry selection rules). Classification of vibrational modes and analysis.
- Orbital Symmetry and Chemical Reactions (Woodward-Hoffman rules for electrocyclic and cycloaddition reactions).

Text Books: F.A. Cotton (Chemical Applications of Group Theory), J.E. Huheey, E.A. Keiter, R.L. Keiter and O.K. Medhi (Inorganic Chemistry: Principles of Structure and Reactivity).
Recommended Books: I. Hargittai and M. Hargittai (Symmetry Through the Eyes of a Chemist), A. Earnshaw (Introduction to Magnetochemistry).

L3 T1 P0 C4

Core Course 202:

Title of the Paper: Organic Chemistry-II

Paper Code: PCHMC-202

Credit: 04

Objectives: Chemistry of natural products, asymmetric synthesis.
Expected Learner Outcome: Understand natural products, methods for asymmetric synthesis.

Unit I: Chemistry of Natural Products (11 Lectures, 15 Marks)

- Terpenoids: Biosynthesis (isoprenoid rule, mevalonic acid pathway), classification, structure elucidation, synthesis of selected mono/sesqui/diterpenes.
- Alkaloids: Classification, extraction, structure elucidation, synthesis of selected alkaloids.

Unit II: Chemistry of Biomolecules (11 Lectures, 15 Marks)

- Carbohydrates: Structure, reaction, conformation of disaccharides (sucrose, maltose, lactose). Polysaccharides (starch, cellulose).
- Peptides and Proteins: Structure determination and synthesis of small peptides (di-, tri-, tetra-). Solid phase peptide synthesis. Classification of proteins (primary, secondary, tertiary structures).

Unit-III: Heterocyclic Chemistry: (13 Lectures, 15 Marks)

- Principles of synthesis (cyclization, cycloaddition).
- Synthesis and properties of three-, four-, and five-membered heterocycles with one/two heteroatoms (N, O, S) like aziridine, oxirane, thiirane, azetidine, oxetane, thietane, pyrazole, isoxazole, isothiazole, imidazole, oxazole, thiazole.

Unit-IV: Mass Spectrometry: (10 Lectures, 15 Marks)

- Ion fragmentation mechanism, Base peak, molecular ion peak, metastable peak, instrumentation, ionization methods, isotopic distribution. Application in determining structure of organic/inorganic compounds.
- Spectroscopic Methods in Analysis**:** Use of IR, electronic, ^{1}H, ^{13}C, ^{31}P NMR, Mass spectrometry in molecular composition/structure analysis.

Text Books: I.L. Finar (Organic Chemistry Vol II), S. Warren (Organic Synthesis: The Disconnection Approach),

L3 T1 P0 C4

Core Course 203:

Title of the Paper: Physical Chemistry-II

Paper Code: PCHMC-203

Credit: 04

Objectives: Understand Schrödinger equation for hydrogen, approximations for complex systems, surface chemistry, and statistical thermodynamics.

Expected Learner Outcome: Students will solve the Schrödinger equation for hydrogen, apply approximations to multi-electron systems, understand surface chemistry concepts, and correlate macroscopic thermodynamic properties with microscopic properties using statistical thermodynamics.

Unit I: Quantum Chemistry II (20 Lectures, 25 Marks)

- Hydrogen atom (Schrödinger equation, radial solution, probability, radial distribution, angular solution, orbitals, degeneracy, angular momentum).
- Approximate methods: Variation theorem, linear variation functions. Time-independent Perturbation theory (non-degenerate, up to second order; application to Helium atom).
- Hellmann-Feynmann theorem. Antisymmetry Principle, Slater determinant, Term symbol, spectroscopic states.
- Born-Oppenheimer approximation, LCAO-MO and VB treatment of H_2 and H_2^+. Comparison of MO and VB methods. Huckel molecular orbital theory (postulates, application to ethylene, butadiene, benzene). Introduction to extended Huckel theory.

Unit II: Surface Chemistry (12 Lectures, 15 Marks)

- Adsorption: Freundlich, Langmuir isotherms, BET theory, physisorption, chemisorption.
- Heterogeneous catalysis (Langmuir-Hinshelwood, Eley-Riedel model, uni/bimolecular surface reaction).
- Colloids: Electrokinetic phenomena, electrical double layer structure, Zeta potential, colloidal stability. Surfactants (definition, classification), micelle formation, Critical Micelle Concentration (CMC). Reverse micelle, solubilization, microemulsion.

Unit III: Statistical Thermodynamics (13 Lectures, 20 Marks)

- Probability, most probable distribution, distinguishable/indistinguishable particles.
- Concept of ensembles, partition functions, distributions (Boltzmann, Fermi-Dirac, Bose-Einstein).
- Ideal gases: Canonical partition function, translational, rotational, vibrational partition functions.
- Absolute thermodynamic quantities (U, H, S, A) for ideal mono/diatomic gases, heat capacity (C_v, C_p), chemical equilibrium.
- Monoatomic Crystals (Einstein and Debye models, T3 dependence of heat capacity). Numerical calculations.

Text Books: P.W. Atkins (Physical Chemistry), I.N. Levine (Physical Chemistry), S. Glasstone (Textbook of Physical Chemistry).

Recommended Books: K.J. Laidler (Chemical Kinetics), D.A. McQuarrie (Statistical Mechanics), A.W. Adamson (Physical Chemistry of Surfaces).

L0 T0 P2 C2

Core Course 204:

Title of the Paper: Chemistry Laboratory-IV

Paper Code: PCHMC-204

Credit: 02

Inorganic Lab II (30 Marks):

- Estimation of Mg^{2+} and Ca2+ by complexometric method.
- Estimation of Zn2+ and Cu2+ by complexometric method in different ores and from given solution with one / two components.
- Estimation of alloys (Brass, Cu-Ni, Bronze).
- Synthesis and characterization of nanoparticles by sol-gel, co-precipitation, and biogenic methods.

L0 T0 P2 C2

Core Course 205:

Title of the Paper: Chemistry Laboratory-V

Paper Code: PCHMC-205

Credit: 02

Organic Lab II (30 Marks):

- Separation and identification of amino acids by paper chromatography.
- Organic Preparation (One-step): Cannizaro reaction of benzaldehyde, oxidation of p-nitrotoluene, reduction of benzophenone, phthalic anhydride to phthalimide.
- Organic Preparation (Two-step): p-nitrobenzene azo 2-naphthol, Benzanilide from benzophenone, Dibenzyl from benzoin.
- Preparation of Green reagent: TetrabutylammoniumTribromide (TBATB) and its use.

L0 T0 P2 C2

Core Course 206:

Title of the Paper: Chemistry Laboratory-VI

Paper Code: PCHMC-206

Credit: 02

Physical Lab II (30 Marks):

- Relative acid strength: Hydrolysis of methyl acetate in HCl and H_2SO_4
- Equivalent conductivity of acetic acid at infinite dilution (Kohlrausch).
- Relative strength of acetic acid and monochloro acetic acid by conductance.
- Specific rotation of sucrose and unknown concentration by polarimetry.
- pH of CH_3COOH and CH_3COONa mixture; dissociation constant.
- Conductometric titration of ternary mixtures (HCl, CH_3COOH, $CuSO_4$; HCl, NaCl, NH_4Cl).
- Ionization constant of acetic acid by conductivity.
- Critical Micelle Concentration (CMC) of SDS by surface tension.

L3 T0 P1 C3

Generic Elective Course 207

Title of the Paper: Materials Chemistry

Paper Code: PCHMG-207

Credit: 04

Objectives: Provide basic knowledge of materials chemistry, classify materials, and understand their synthesis, properties, and applications.
Expected Learner Outcome: Comprehend different types of materials, their synthesis, characterization, and applications.

Unit I: Introduction to Materials (10 Lectures, 10 Marks)

- Classification of materials (metals, ceramics, polymers, composites), bonding in materials.
- Crystalline and amorphous solids, defects in solids, crystal structures (BCC, FCC, HCP).

Unit II: Advanced Materials (20 Lectures, 20 Marks)

- Nanomaterials: Synthesis (top-down, bottom-up), characterization, properties, applications.
- Smart materials: Shape memory alloys, pH-sensitive materials, self-healing materials.
- Biomaterials: Biocompatibility, types, applications in medicine.

Unit III: Polymer Materials (20 Lectures, 30 Marks)

- Historical background, basic nature, classification, raw materials, gas cracker, naphtha cracker, Molecular forces and chemical bonding in polymers, Texture of Polymers.
- Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.
  Physical, thermal, Flow & Mechanical Properties of polymers. Conducting polymers-Introduction, conduction mechanism, polyaniline (PANI), polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications.polymer-matrix composites. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Text Books: W.D. Callister (Materials Science and Engineering: An Introduction), C.N.R. Rao and B. Raveau (Transition Metal Oxides), A.R. West (Solid State Chemistry and its Applications).

Recommended Books: M. Faraday (Experimental Researches in Chemistry and Physics), J. Zarzycki (Glasses and the Vitreous State), L.V. Azaroff (Introduction to Solids);Inorganic Chemistry, Shriver & Atkins, 5th Edition Oxford; Introduction to Polymer by R. J. Young and P. A. Lovell

Semester III

Detailed Syllabus - Semester III: **L3 T1 P0 C4**

Core Course 301:

Title of the Paper: Inorganic Chemistry-III

Paper Code: PCHMC-201

Credit: 04

Objectives: Knowledge about properties of d and f block elements and spectroscopic methods in Inorganic Chemistry.

Expected Learner Outcome: Students will solve spectroscopic problems for inorganic molecules and gather thorough knowledge about the chemistry of d and f block elements.

Unit I: Properties of Transition Metal Complexes (15 Lectures, 17 Marks)

- Donor-acceptor compounds, coordination number and geometries, 18-electron rule, stability (thermodynamic vs. kinetic), common ligands and complexes, stereochemical non-rigidity.
- Chemistry of Lanthanides and Actinides: Properties (magnetic and spectral), separation, lanthanide shift reagents. Stability of lanthanide/actinide complexes.

Unit II: Introduction to Organotransition Metal Chemistry (10 Lectures, 13 Marks)

- Metal-carbon bond formation, 18 and 16 electron organometallic complexes. Isolobal analogy.
- Bonding (metal carbonyls, olefins, carbenes), role of co-ligands (phosphine, arsine, stibine, N_2, O_2, NO). Oxidative addition, reductive elimination, β-elimination.

Unit III: Spectroscopic methods in Inorganic Chemistry (20 Lectures, 30 Marks)

- Electronic Spectra and Magnetic Properties: Electronic states and terms. Selection rules. Orgel and Tanabe-Sugano diagrams (application). d-d and charge transfer transitions. Magnetic properties based on crystal field theory (spin only moments, spin-state equilibrium, orbital contribution, temperature effect).
- Application of NMR Spectroscopy (^{1}H, ^{31}P, ^{19}F): Chemical shift, factors, spin-spin coupling Use in coordination chemistry (metal-ligand interaction, isomer determination, stereochemical non-rigidity).
- ESR Spectroscopy: Spin orbit coupling, Kramer degeneracy, zero-field splitting, hyperfine and superhyper interaction, line width. Application in organic radicals and transition metal complexes (d^1, d^3, d^9).
- Mössbauer Spectroscopy: Principle, instrumentation. Applications: isomer shift, magnetic interaction, quadrupole splitting, line width. Application to iron and tin compounds.
- Introduction to NQR Spectroscopy & Photoelectron Spectroscopy

Text Books: R.H. Crabtree (The Organometallic Chemistry of the Transition Metals), J.P. Collman, L.S. Hegedus, J.R. Norton, R.G. Finke (Principles and Applications of Organotransition Metal Chemistry).
Recommended Books: A. Yamamoto (Organotransition Metal Chemistry: Fundamental Concepts and Applications), C. Elschenbroich, A. Salzer (Organometallics – A Concise Introduction).

L3 T1 P0 C4

Core Course 302:

Title of the Paper: Organic Chemistry-III

Paper Code: PCHMC-302

Credit: 04

Objectives: Impart basic knowledge on conformational behavior, asymmetric synthesis and redox reagents.

Expected Learner Outcome: Students will understand basics of gain stereochemical insight, methods for asymmetric synthesis and become familiar with various oxidative and reductive reagents.

Unit I: Stereochemistry II (Conformation) (12 Lectures, 16 Marks)

- Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-, 3-, 4-alkyl ketone effects.
- A1,2 and A1,3 strains. Conformation of fused systems (decalins, perhydrophenanthrenes).
- Effects of conformation on reactivity/mechanism of 6-membered ring compounds. Chiroptical properties (ORD, CD, axial haloketone rule, octane rule).

Unit II: Asymmetric Synthesis (10 Lectures, 15 Marks)

- Catalytic asymmetric synthesis: Sharpless epoxidation, Sharpless asymmetric dihydroxylation, CBS reduction, Jacobsen epoxidation, asymmetric hydrogenation.
- Chiral auxiliary-based asymmetric synthesis: Alkylation, Diels-Alder reaction, Aldol reaction.

Unit III: Oxidation (10 Lectures, 13 Marks)

- Carbon-Carbon Double Bond: Dihydroxylation by $KMnO_4$, OsO_4 (Sharpless asymmetric dihydroxylation), iodine and silver carboxylate (Woodward and Prevost), peroxy acid. Allylic and benzylic oxidation (SeO_2, DDQ).
- Alcohols: Cr(VI) based reagents (PCC, PDC), DMSO-based reagents (Swern, Pfitzner-Moffatt, Albright-Goldman), Tetrapropyl ammonium perruthenate (TPAP). 1,2-diols.

Unit IV: Reduction (13 Lectures, 16 Marks)

- Catalytic Hydrogenation: Heterogeneous (H_2/Pd-C, H_2/Pt_2O, Lindlar's, Rosendmund's), homogeneous (Wilkinson catalyst).
- Modified Hydride Transfer Reagents: Lithium trialkoxyaluminium hydrides, DIBAL, $NaCNBH_4$, SMEAH (Red Al), Superhydride, Selectrides, 9-BBN.
- Dissolving Metal: Alkali metals in liquid ammonia.
- Diimide.
- Electrooxidation and reduction. Use of Baker's Yeast.

L3 T1 P0 C4

Core Course 303:

Title of the Paper: Physical Chemistry-III

Paper Code: PCHMC-303

Credit: 04

Objectives: Impart knowledge on reaction kinetics, electrochemistry, and solid-state chemistry.

Expected Learner Outcome: Students will understand reaction kinetics, solve problems in galvanic/electrolytic cells, grasp ion-ion/ion-solvent interactions, and learn about crystalline solids, defects, and band theory applications.

Unit I: Advanced Chemical Kinetics (18 Lectures, 23 Marks)

- Complex reactions: Chain reactions (thermal, photochemical), explosion limits.
- Theories of reaction rates: Collision theory, Transition state theory, unimolecular reactions (Lindemann, Hinshelwood, Slater's, RRKM).
- Methods of studying fast reaction (flow method, temperature/pressure jump, NMR, flash photolysis, femto-chemistry).
- Reactions in solutions: Effect of pressure, ionic strength, dielectric constant.
- Homogeneous catalysis: Acid-base catalysis (specific, general), enzyme catalysis (Michaelis-Menten).
- Electrochemical kinetics: Butler-Volmer equation, Tafel equation, overpotential, current density.

Unit II: Advanced Electrochemistry (17 Lectures, 22 Marks)

- Introduction to electrochemistry (galvanic/electrolytic cells, electrode kinetics, dynamic electrochemistry, mass transport by migration/diffusion/convection, diffusion layers).
- Ion-Solvent Interaction, Ion-Association (Bjerrum's hypothesis, Thermodynamics of ion-pairing, Debye-Huckel free ion and Bjerrum's ion-pair).
- Polarizable/non-polarizable electrodes. Inner and Outer potential.
- Thermodynamics of Electrified Interfaces (Surface Excess, relevance of outer/surface potential to double layer (DL) studies, surface/inner potential difference). Capacity potential relations in electrode-electrolyte interface, Contact adsorption. Electrical double layer (HP/GC/Stern model).
- Electrocatalysis (definitions, potential, effect of electric field). Nanostructured and surface modified electrodes. Introduction to batteries, fuel cells, electrochemical solar cells.

Unit III: Condensed Systems (10 Lectures, 15 Marks)

- Liquid state: Structure of liquids, theories of liquid state (Eyring, free volume), transport properties (viscosity, diffusion).
- Liquid crystals: Nematic, smectic, cholesteric phases, properties, applications.

- Solid state: Crystal symmetry, band theory of solids, semiconductors, superconductors, defects.

Text Books: A.W. Adamson (Physical Chemistry of Surfaces), N.B. Hannay (Solid State Chemistry), R. Chang (Physical Chemistry for the Chemical and Biological Sciences).
Recommended Books: G.A. Somorjai (Introduction to Surface Chemistry and Catalysis), C. Kittel (Introduction to Solid State Physics), P.W. Atkins (Physical Chemistry).

L0 T0 P2 C2

Core Course 304:

Title of the Paper: Chemistry Laboratory-VII

Paper Code: PCHMC-304

Credit: 02

Inorganic Lab III (30 Marks):

- Synthesis and characterization (melting point, conductivity, IR, UV-vis) of trans-triglycinatoCu(II) monohydrate (and Ni-DMG complex); estimate percentage of Cu (Ni).
- Synthesis and characterization of Schiff-base ligands and their metal complexes.
- Synthesis and characterization of magnetic nanoparticles by surfactant assisted methods.

L0 T0 P2 C2

Core Course 305:

Title of the Paper: Chemistry Laboratory-VIII

Paper Code: PCHMC-305

Credit: 02

Organic Lab III (30 Marks):

- Preparation, purification (by TLC), and spectroscopic identification (UV, IR) of prepared organic compounds.
- Preparations: Benzilic acid from benzoin; Benzanilide from benzophenone; Indigo from anthranilic acid; Sandmeyer reaction (ortho-Chlorotoluene, Acridone); Sulphanilamide from acetanilide; Pinacolone from benzophenone.
- Estimation: Glycine by formalin method; halogen by fusion; hydroxyl/amino groups by acetylation.
- Synthesis of Deep Eutectic Solvents (DES) and its use.
- Green synthesis of Coumarin derivative (clay catalyzed).
- Benzoin condensation using Green catalysts (co-enzymes).

L0 T0 P2 C2

Core Course 306:

Title of the Paper: Chemistry Laboratory-IX

Paper Code: PCHMC-306

Credit: 02

Physical Lab III (30 Marks):

- Hydrolysis constant of aniline hydrochloride by pH measurements.
- Strengths of mixtures by conductometric titration (HCl, CH_3COOH; H_2SO_4, CuSO4).
- Strengths of HCl and CH_3COOH by pH-metric titration.
- Verify Beer's law and determine unknown concentration (KMnO4, $K_2Cr_2O_7$).
- Composition of iron-salicylic acid complex spectrophotometrically by Job's method.
- Least squares fitting and plotting linear/exponential graphs using computer.
- Composition of binary mixture ($K_2Cr_2O_7$ and $KMnO_4$) by spectroscopic method.
- Indicator constant of methyl red.
- Reaction between H_2O_2 and HI (clock reaction), activation energy.
- Molecular surface energy and association factor for ethanol.
- Spectroscopic properties of acetone in different solvents, hydrogen bonding energy.

L0 T0 P2 C2

Discipline Specific Elective Course 308:

Title of the Paper: Project-I

Paper Code: PCHMD-308

Credit: 02

Objective: This project-based course aims to equip M.Sc. Chemistry students with the essential skills required for advanced scientific communication, specifically through the rigorous process of writing a review article.

Expected Learner Outcome: Upon completion of this course, students will be able to formulate a focused research question or topic suitable for a comprehensive literature review in a specific area of Chemistry.

Description: During this project work student will have to learn Scientific Literature survey methods including literature search strategies and databases, bibliographic management tools (e.g., Mendeley/Zotero) and write a review article which have to be communicated for journal publication.

The project will be assessed based on Presentation (30 marks) and the report (20 Marks).

L2 T0 P0 C2

Ability Enhancement Course 309:

Title of the Paper: Analytical Chemistry-I

Paper Code: PCHMA-309

Credit: 02

Objectives: Instrumentation of UV-Visible spectrometry, FT-IR, principles of Thermal methods, Polarography, powder and single crystal XRD. Understand applications of these techniques.

Expected Learner Outcome: Knowledge of instrumental parts, working principles, applications, and characterization/analysis skills using these techniques.

Unit I (15 Lectures, Marks 15):

- Instrumentation and application of UV-Visible, IR, BET.
- Principles and applications of powder and single crystal XRD.
- Electron Microscopy (SEM, TEM): Principles, imaging, elemental analysis.

Unit II (15 Lectures, Marks 15):

- Polarography: principles, instrumentation, applications of cyclic voltammetry.
- Thermal methods: principles and applications of TG, DTG, DTA, DSC.

Text Books: H Kaur (Instrumental Methods of Chemical Analysis).
Recommended Books: A. R. West (Solid State Chemistry and its Applications), M.E. Brown (Introduction to Thermal Analysis: Techniques and Applications).

L3 T1 P0 C4

Semester IV

Core Course 401:

Title of the Paper: Research Methodology & Green Chemistry

Paper Code: PCHMC-401

Credit: 04

Objectives: Understand research process, scientific data analysis, green chemistry practices.

Expected Learner Outcome: Students will gain knowledge about the research process, analyze data scientifically, and design greener methodologies.

Unit I: Research Methodology (15 Lectures, 20 Marks)

- Meaning, objective, motivation, types of research, methods vs. methodology.
- Research process (defining problem, literature survey, hypothesis, design, sampling, data collection).
- Data analysis (measures of central tendency/dispersion/asymmetry/relationship).
- Regression analysis, t-test, p-test. Citations, impact factors, author index.

Principles of Green Chemistry and Designing a Chemical Synthesis (10 Lectures, 12 Marks)

- What is Green Chemistry? Need, Goals, Limitations, Obstacles; E-factor.
- Twelve principles (waste prevention, atom economy, hazardous product minimization, green solvents, energy sources, starting materials, catalytic reagents, accident prevention).
- Bioctalysis, Photocatalyzed reactions.

Examples of Green Reagents/Synthesis/Reactions (20 Lectures, 28 Marks)

- Green synthesis (adipic acid, catechol, disodium iminodiacetate, paracetamol, ibuprofen).
- Microwave assisted reactions (in water, organic solvents, solvent-free - Michael addition, Knoevenagel).
- Ultrasound assisted reactions (Grignard, Ulmann coupling, Cannizaro).
- Dimethyl carbonate (DMC), TetrabutylammoniumTribromide (TBATB), Rongalaite as green reagents.
- Oxidation reagents and catalysts; Biomimetic multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions.
- Cocrystal Controlled Solid-State Synthesis (C3S3).

Text Books: C.R. Kothari and Gaurav Garg (Research Methodology Methods and Techniques), P.T. Anastas & J.K. Warner (Oxford Green Theory and Practical).

Recommended Books: A.S. Matlack (Introduction to Green Chemistry), M.C. Cann & M.E. Connely (Real-World cases in Green Chemistry), M.A. Ryan & M. Tinnesand (Introduction to Green Chemistry).

In Semester IV, students will specialize in one of the following branches: Inorganic, Organic, or Physical Chemistry.

Specialization Options in Semester IV:

Detailed Syllabus - Inorganic Chemistry Specialization:

Discipline Specific Elective Course 402: **L3 T1 P0 C4**

Title of the Paper: Inorganic Chemistry-IV (Special Topics in Inorganic Chemistry)

Paper Code: PCHMD-402

Credit: 04

Objectives: Advanced topics in inorganic chemistry, including supramolecular chemistry, materials, and photochemistry.

Expected Learner Outcome: Understanding of non-covalent interactions, MOFs, COFs, inorganic host-guest systems, and inorganic photochemistry.

Unit I: Supramolecular Chemistry (12 Lectures, 17 Marks)

- Non-covalent forces: Hydrogen bonding, van der Waals forces, π-π interactions, host-guest chemistry.
- Molecular recognition, self-assembly, supramolecular architecture.
- Crown ethers, cryptands, cyclodextrins, calixarenes.

Unit II: Inorganic Materials (20 Lectures, 25 Marks)

- Solid state ionic conductors: Structure, physico-chemical principles, applications. Ferrous alloys, Fe-C phase transformations in ferrous alloys; non-ferrous alloys-properties and applications, magnetic alloy. Metallic glass, ceramics.
- Inorganic Polymers: Polysiloxanes, polysilanes, polyphosphazenes, polymeric sulphur- synthesis, structure, properties and applications. co-ordination polymers and organometallic polymers.
- Metal-Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs): Synthesis, structure, applications.
- Inorganic host materials: Zeolites, clays, layered double hydroxides.
- Nanomaterials: Quantum dots, nanoparticles, nanowires, carbon nanotubes.

Unit III: Inorganic Photochemistry and Catalysis (13 Lectures, 18 Marks)

- Excited states, ligand field states, charge-transfer states, Thexi states; phosphorescence, fluorescence; photochemical reactions.
- Photoinduced electron transfer, energy transfer, luminescence.
- Photochemical reactions involving inorganic complexes and redox active centers.
- Photocatalysis for water splitting, semiconductors, dye sensitized solar cell, Ru-complexes, role of co-catalysts.

Text Books: J.W. Steed and J.L. Atwood (Supramolecular Chemistry), O.M. Yaghi, M. O'Keeffe, N.W. Ockwig, H.K. Chae, M. Eddaoudi, J. Kim (Reticular Chemistry: Structure, Properties, and Applications).
Recommended Books: V. Balzani and F. Scandola (Supramolecular Photochemistry), G.A. Ozin and A.C. Arsenault (Nanochemistry: A Chemical Approach to Nanomaterials).

Discipline Specific Elective Course 403: **L3 T1 P0 C4**

Title of the Paper: Inorganic Chemistry-V (Bio-Inorganic Chemistry)

Paper Code: PCHMD-403

Credit: 04

Objectives: Comprehensive understanding of inorganic elements in biological systems.
Expected Learner Outcome: Knowledge of metal ions in biological processes, metalloproteins, and medicinal inorganic chemistry.

Unit I: Metal Ions in Biological Systems (25 Lectures, 30 Marks)

- Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins. Role in muscle contraction, blood clotting mechanism and biological calcification. Na-K pump.
- Proteins and enzymes of Fe, Co, Cu, Mo and Zn: Hemerythrin, ferritin and transferrins, peroxidase, catalase, cytochrome P-450. Cytochrome C oxidase and superoxide dismutase, ceruloplasmin, Vitamin B_{12}, B_{12} co-enzymes and cobalamines, carbonic anhydrase, carboxy peptidase, metallothionins, interchangeability of Zn and Co in enzymes.
- Structural and functional models, Biological nitrogen fixation.
- Metals in medicine: Toxicity of mercury, cadmium, lead, chromium, beryllium, selenium and arsenic, biological defence mechanisms, chelation therapy, metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

Unit II: Electron Transfer and Enzymes (10 Lectures, 15 Marks)

- Electron transfer proteins: Cytochromes, iron-sulfur proteins, blue copper proteins.
- Metalloezymes: Carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, nitrogenase, superoxide dismutase.
- Bio-mimetic chemistry: Synthetic models of metalloenzymes.

Unit III: Medicinal Inorganic Chemistry (10 Lectures, 15 Marks)

- Metal-based anticancer drugs (cisplatin and its analogs).
- Metal complexes as diagnostic agents (MRI contrast agents, radiopharmaceuticals).
- Chelation therapy, metal toxicity.

Text Books: I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine (Bioinorganic Chemistry), R.W. Hay (Bio-inorganic Chemistry).
Recommended Books: J.A. Cowan (Inorganic Biochemistry - An Introduction), W. Kaim, B. Schwederski (Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life).

Detailed Syllabus - Organic Chemistry Specialization:

L3 T1 P0 C4

Discipline Specific Elective Course 404:

Title of the Paper: Organic Chemistry-IV (Methods in Organic Synthesis)

Paper Code: PCHMD-404

Credit: 04

Objectives: Modern synthetic methodologies and reagents in organic chemistry.
Expected Learner Outcome: Proficiency in designing and executing complex organic syntheses.

Unit II: Carbon-Carbon Bond Formation (10 Lectures, 15 Marks)

- Coupling reactions: Heck, Suzuki, Sonogashira, Stille, Negishi, Buchwald-Hartwig.
- Enamine and enolate chemistry, aldol and Claisen condensations, Michael addition.
- Wittig reaction, Horner-Wadsworth-Emmons reaction, Baylis-Hillman reaction.

Unit II: Photochemistry of Organic Compounds (20 Lectures, 25 Marks)

- Jablonski diagram, photosensitization, quenching.
- Olefinic photochemistry (Photostereomutation of cis-trans isomers, optical pumping, photochemistry of conjugated dienes - cycloaddition, dimerization of butadiene, Photochemistry of vision).
- Photochemistry of carbonyl compounds (Norrish type I and type II processes, photoreduction of saturated aryl, alkyl and unsaturated ketones, Paterno-Buchi reaction).
- Photorearrangements (di-π-methane rearrangement, rearrangement of cyclohexadienes). Reaction of singlet oxygen, photooxidation.

Unit III: Rearrangements and Pericyclic Reactions (15 Lectures, 20 Marks)

- Rearrangements involving electron deficient carbon (Wagner-Meerwein), nitrogen (Hoffmann, Curtius, Schmidt), oxygen (Baeyer-Villiger).
- Pericyclic reactions: Classification, FMO method, Orbital symmetry correlation method, PMO method (thermal, photochemical conditions).

- Cycloaddition reactions ([2+2], [4+2], [6+4]), 1,3-dipolar cycloadditions; ene reaction, cheletropic reactions.
- Sigmatropic rearrangement ([m+n] shifts of hydrogen and carbon), Cope and Claisen rearrangement.
- Electrocyclic reactions. Stereoselectivity and regioselectivity.

Text Books: M.B. Smith (Organic Synthesis), J. Clayden, N. Greeves, S. Warren (Organic Chemistry).
Recommended Books: R. Larock (Comprehensive Organic Transformations), L. Kurti, B. Czako (Strategic Applications of Named Reactions in Organic Synthesis).

Discipline Specific Elective Course 405: **L3 T0 P0 C4**

Title of the Paper: Organic Chemistry-V (Heterocyclic Compounds and Medicinal Applications)

Paper Code: PCHMD-405

Credit: 04

Objectives: Comprehensive knowledge of heterocyclic compounds and their applications in medicinal chemistry.
Expected Learner Outcome: Understanding of synthesis, reactions, and medicinal importance of various heterocyclic systems.

Unit I: Five-membered Heterocycles (12 Lectures, 15 Marks)

- Pyrrole, furan, thiophene: Synthesis, reactivity (electrophilic substitution), aromaticity.
- Indole, benzofuran, benzothiophene: Synthesis and reactions.
- Pyrazol, imidazole, oxazole, thiazole: Synthesis and reactions.

Unit II: Six-membered Heterocycles (13 Lectures, 15 Marks)

- Pyridine, quinoline, isoquinoline: Synthesis, reactivity, aromaticity.
- Diazines (pyridazine, pyrimidine, pyrazine): Synthesis and reactions.
- Pteridines, purines, pyrimidines (related to nucleic acids).

Unit III: Medicinal Chemistry (20 Lectures, 30 Marks)

- Drugs: Definition of drugs, factors affecting bioactivity. Chemotherapeutic index, therapeutic index.
- Quantitative structure activity relationship (QSAR). Drug receptor concepts, theoretical aspects of drug-receptor interaction. Drug introduction, Metabolism, Excretion.
- Introduction to drug designing; Structural modification of drugs. Combinatorial library of drugs.

- Sulphadrugs: Historical significance, Sulphanilamide and other important sulpha drugs, mode of action.
- Antibiotics: Introduction, classification, structure-action relationship, mode of action of penicillin, semisynthetic penicillins, streptomycin, tetracyclins.
- Antimalarials: Introduction, classification, human malaria and plasmodia, mepaquine, trimethoprim, mefloquine (structure and activity). Artemisinin and derivatives, structure-action relationship.
- Drugs for Cancer and Tuberculosis: Recent developments.

Text Books: T.L. Gilchrist (Heterocyclic Chemistry), G.L. Patrick (An Introduction to Medicinal Chemistry).
Recommended Books: J.A. Joule and K. Mills (Heterocyclic Chemistry), D. Lednicer (The Organic Chemistry of Drug Synthesis).

Detailed Syllabus - Physical Chemistry Specialization:

Discipline Specific Elective Course 406: **L3 T1 P0 C4**

Title of the Paper: Physical Chemistry-IV (Computational Chemistry and Numerical Analysis)

Paper Code: PCHMD-406

Credit: 04

Objectives: Introduction to computational chemistry, quantum chemical methods, and numerical analysis.
Expected Learner Outcome: Understanding of computational approaches to chemical problems and basic numerical methods.

Unit I: Quantum Chemical Methods (20 Lectures)

- Hartree-Fock theory: Roothaan equations, basis sets.
- Post-Hartree-Fock methods: Configuration Interaction (CI), Møller-Plesset perturbation theory (MPn).
- Density Functional Theory (DFT): Basic theorems, exchange-correlation functionals, applications.

Unit II: Molecular Mechanics and Dynamics (15 Lectures, 20 Marks)

- Molecular mechanics: Force fields, energy minimization.
- Molecular dynamics simulations: Ensembles, integration algorithms, applications.
- Monte Carlo simulations.

Unit III: Numerical Methods (10 Lectures, 15 Marks)

- Solving ordinary and partial differential equations.

- Matrix operations, interpolation, curve fitting, numerical integration.

Text Books: A.R. Leach (Molecular Modelling: Principles and Applications), J.B. Foresman and A. Frisch (Exploring Chemistry with Electronic Structure Methods).
Recommended Books: C. Cramer (Essentials of Computational Chemistry: Theories and Models), D.C. Young (Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems).

L3 T1 P0 C4

Discipline Specific Elective Course 407:

Title of the Paper: Physical Chemistry-V (Organic Solid States Chemistry / Chemistry of Materials)

Paper Code: PCHMD-407

Credit: 04

Core 406:

Objectives: Concepts of dynamic electrochemistry, solid state electrochemistry, electrocatalysis, and advanced materials chemistry.
Expected Learner Outcome: Understanding of electrochemical processes, non-equilibrium thermodynamics, and properties of various materials.

Unit I: Advanced Electrochemistry (20 Lectures, 30 Marks)

- Introduction (Nernst equation, electrode kinetics, dynamic electrochemistry, Butler-Volmer and Tafel equations), Overpotentials.
- Kinetically and mass transport-controlled processes. Mass transport by migration, convection, diffusion. Conductivity.
- Solid-state electrochemistry. Ion-conducting and electronically conducting polymers. Electrochemical double layer.
- Potentiostatic and galvanostatic electrochemical methods (chronoamperometry, coulometry, cyclic voltammetry, impedance spectroscopy). Thermodynamics of Electrocapillary phenomenon; Surface excess, relevance of outer/surface potential to double layer (DL) studies. Capacity potential relations, contact adsorption.
- Electrocatalysis (definitions, potential, effect of electric field). Nanostructured and surface modified electrodes.
- Introduction to batteries, fuel cells, electrochemical solar cells. Electrochemical processes for energy conversion.

Unit II: Non-Equilibrium Thermodynamics and Transport Phenomena (15 Lectures, 18 Marks)

- Difference between equilibrium and non-equilibrium thermodynamics.
- Criteria of non-equilibrium thermodynamics; Assumptions, uncompensated heat.
- Fluxes and forces (linear laws, Onsager relation, microscopic reversibility, Onsager reciprocity). Coupled reaction.

- Thermoelectric effects (Seebeck, Peltier, Thompson).

Unit III: Chemistry of Materials (10 Lectures, 12 Marks)

- Organic solids: Conducting organics, organic superconductors, magnetism in organic materials.
- Fullerenes: doped fullerenes as superconductors.
- Molecular devices: rectifiers, transistors, artificial photosynthetic devices, sensors.
- Clay-polymer composite and carbon composites, phosphor and laser materials.

Text Books: J.O.M. Bockris and A.K.N. Reddy (Modern Electrochemistry), S.R. de Groot and P. Mazur (Non-Equilibrium Thermodynamics).
Recommended Books: A. Bard and L. Faulkner (Electrochemical Methods: Fundamentals and Applications), F. Haase and S. Haase (Thermodynamics of Irreversible Processes).

Discipline Specific Elective Course 408: **L0 T0 P4 C4**

Title of the Paper: Project-II

Paper Code: PCHMD-408

Credit: 04

PR 408: Project-II

Objectives: This project-based course is designed to provide M.Sc. Chemistry students with hands-on experience in independent scientific research, culminating in a laboratory-based project and dissertation.

Expected Learner Outcome: Develop independent research capabilities, problem-solving skills, and the ability to contribute to scientific knowledge.

Description: Students will undertake an independent research project under the supervision of a faculty member. The project will involve literature review, experimental work (or theoretical/computational studies), data analysis, and preparation of a detailed dissertation report. A viva-voce examination will be conducted based on the dissertation.

Marks Distribution: Dissertation (90 Marks), Viva-voce (30 Marks), Internal Assessment (80 Marks).

Ability Enhancement Course 409:

Title of the Paper: Analytical Chemistry-II **L2 T0 P0 C2**

Paper Code: PCHMA-409

Credit: 02

Objectives: Advanced analytical techniques for chemical analysis.
Expected Learner Outcome: Proficiency in advanced analytical instrumentation and their applications.

Unit I: Separation Techniques (10 Lectures, 10 Marks)

- Chromatography: HPLC, GC, Ion Chromatography, Capillary Electrophoresis. Principles, instrumentation, applications.

Unit II: Spectroscopic Techniques (10 Lectures, 10 Marks)

- Atomic absorption spectroscopy (AAS), Atomic emission spectroscopy (AES), Inductively Coupled Plasma (ICP) techniques.
- X-ray fluorescence (XRF), Neutron Activation Analysis (NAA).
- Mass Spectrometry (MS): Principles, ionization techniques, analyzers, applications.

Unit III: Electroanalytical Techniques (10 Lectures, 10 Marks)

- Voltammetry (linear sweep, cyclic), Amperometry, Coulometry, Potentiometry (ion-selective electrodes).

Text Books: D.A. Skoog, F.J. Holler, S.R. Crouch (Principles of Instrumental Analysis), G.D. Christian, P.K. Dasgupta, K.A. Schug (Analytical Chemistry).
Recommended Books: R.L. Grob and E.F. Barry (Modern Practice of Gas Chromatography), J. Dean (Analytical Chemistry Handbook).