Darrang College (Autonomous), Tezpur-784001

Syllabus

Two year Post Graduate Course

(As per National Education Policy, 2020)

Subject: Chemistry

Approved by:

Board of Studies meeting held on 10-06-2026 &

Academic Council vide Resolution no. DC/AC/3/2026/06 dated 29th June 2026

Curriculum Structure for 2 Year PG Programme

M.Sc. Semester-1				
Course Type	**Course**	**Course code**	**Credit**	**L-T-P**
Core	Inorganic Chemistry-I	CHE-1-DSC-4014	4	3-0-1
Core	Organic Chemistry-I	CHE-1-DSC-4024	4	3-0-1
Core	Physical Chemistry-I	CHE-1-DSC-4034	4	3-0-1
DSE	Quantum Chemistry	CHE-1-DSE-4044 (A)	4	3-0-1
DSE	Polymer Chemistry	CHE-1-DSE-4044 (B)	4	3-0-1
FSC	Research Methodology (Swayam)	CHE-1-FSC-4054	4	4-0-0
M.Sc. Semester-2				
Core	Inorganic Chemistry-II	CHE-2-DSC-5014	4	3-0-1
Core	Organic Chemistry-II	CHE-2-DSC-5024	4	3-0-1
Core	Physical Chemistry-II	CHE-2-DSC-5034	4	3-0-1
DSE	Spectroscopy	CHE-2-DSE-5044(A)	4	3-0-1
DSE	Petroleum Science and Technology	CHE-2-DSE-5044(B)	4	3-0-1
FSC	Analytical and Computational Chemistry	CHE-2-FSC-5054	4	3-0-1
M.Sc. Semester-3				
Core	Foundations of Organic synthesis and Green Chemistry	CHE-3-DSC-5064	4	3-0-1
Core	Materials Chemistry	CHE-3-DSC-5074	4	3-0-1
Core	Surface Chemistry and Catalysis	CHE-3-DSC-5084	4	3-0-1
Core	Advanced Bioinorganic Chemistry	CHE-3-DSE-5094	4	3-0-1
Elective	Supramolecular Chemistry	CHE-3-DSC-5104(A)	4	3-0-1
Elective	Biochemistry	CHE-3-DSE-5104(B)	4	3-0-1
M.Sc. Semester-4 (Research)				
Core	Dissertation	CHE-4-PRJ-511-20	20	0-0-20

Program Specific Outcomes (PSOs)

- **PSO 1:** Demonstrate comprehensive mastery of advanced theoretical frameworks and reaction mechanisms across Organic, Inorganic, Physical, and Analytical chemistry.
- **PSO 2:** Acquire specialized proficiency in operating sophisticated analytical instrumentation and executing complex structural elucidation (NMR, FTIR, MS, HPLC).
- **PSO 3:** Formulate hypotheses, design rigorous experimental methodologies, and apply critical cognitive skills to analyze data and solve advanced chemical problems.
- **PSO 4:** Evaluate environmental impacts and integrate green chemistry principles to design sustainable, eco-friendly chemical processes and synthetic pathways.
- **PSO 5:** Apply core chemical principles to emerging interdisciplinary sectors, including nanotechnology, materials science, and pharmaceutical engineering.
- **PSO 6:** Draft and deliver professional, high-quality scientific communications, including technical research reports, grant proposals, and academic presentations.
- **PSO 7:** Uphold rigorous standards of research bioethics, enforce stringent laboratory safety and waste-management protocols, and commit to continuous professional development.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
1	CHE-1-DSC-4014	Inorganic Chemistry-I	3	1	4

Course Outcomes (COs)

- **CO1:** Explain the fundamentals of group formation.
- **CO2:** Classify molecules on the basis of their symmetry.
- **CO3:** Develop molecular orbitals for complexes.
- **CO4:** Explain bonding in coordination compounds.
- **CO5:** Analyze magnetic properties of inorganic compounds.

Theory (45 Hours)

Unit 1. Molecular Symmetry and the Symmetry Groups (4h)

- Symmetry elements and operations
- Classes of symmetry operations, symmetry and chirality
- Symmetry point groups

Unit 2. Representation of Groups (6 h)

- Matrix notation for geometric transformations, reducible and irreducible representations,
- Rules about irreducible representation as derived from great orthogonality theorem
- Relationship between reducible and irreducible groups
- Character tables

Unit 3. Chemical Applications of Group Theory (13 h)

- Group Theory and Quantum Mechanics - wave functions as bases for irreducible representations,
- Direct product and its importance in predicting spectral transition probabilities.
- Symmetry properties of atomic orbitals
- Molecular orbitals for σ and π bonding in AB_4 and AB_6
- Ligand field states, construction of the correlation diagram for the d^2 configuration in an octahedral environment.

Unit 4. Orbital splitting and electronic Spectra of coordination Compounds (12 h)

- CFT, d-orbital splitting in coordination complexes with different symmetries
- Jahn-Teller distortion, CFSE for d^1 to d^{10} systems and pairing energy
- Low-spin and high-spin complexes
- *d-d* transition, charge transfer transition, color, intensity and origin of spectra
- Interpretation, term symbols and splitting of terms different geometries
- Selection rules for electronic transitions, correlation
- Tanabe-Sugano and Orgel diagrams, calculation of Dq, B and C, nephelauxetic ratio.

Unit 5. Magnetic Properties (10 h)

- Magnetic properties of free ions

- Types of magnetic behaviour: dia-, para-, ferro- and antiferro-magnetism
- Temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation
- Magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling
- Magnetic properties of second and third transition series and lanthanides

Laboratory (30 Hours)

1. Molecular orbital calculations of simple inorganic compounds.
2. Density Functional Theory (DFT) calculations for the analysis of Normal Modes (IR and Raman Vibrations).
3. Preparation of bis(*N*,*N*-disalicylideneethylenediammine) and bis(*N*,*N*-disalicylideneethylenediammine) (μ-aquadicobalt(II)). UV-Vis. and IR Characterization.
4. Preparation of *cis*- and *trans*-bisglycinatocopper(II) complex. UV-Vis. and IR Characterization.
5. Solution phase synthesis of co-ordination compounds e.g. vanadylacetylacetonato, trioxalatometal (III)trihydrates etc. (characterization, properties and applications).
6. Determination of magnetic moments of inorganic complexes by using Gouy balance.
7. Determination of Electronic Spin Configuration via Evans Method (magnetic moment measurement).

Books Recommended:

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edition, Willey India Pvt. Ltd. 2008.
2. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1998
3. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, 4th Ed. Pearson Education, 2006.
4. B. N. Figgis, M. A. Hitchman; Ligand Field theory and its Applications, Wiley India, 2010.
5. G. L. Miessler, D Tarr; Inorganic Chemistry. 3rd Ed., Pearson Education, 2004.
6. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver & Atkins 'Inorganic Chemistry, 5th Ed. Oxford University Press, 2010.
7. Fundamental Concepts of Inorganic Chemistry, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015.
8. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, 2nd Ed. Affiliated East-West Press Pvt. Ltd.-New Delhi, 2004.
9. F. E. Mabbs, D. J. Machin, Magnetism and Transition Metal Complexes, Dover Pub. Inc., 2008.
10. Reaction Mechanism in Inorganic Chemistry 2nd Ed. R. R. Jordan Oxford University Press, 1998.
11. F. Basolo, R. G. Pearson, Mechanism of Inorganic Reactions 2nd Ed. Wiley Eastern Pvt. Ltd. 1973

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
1	CHE-1-DSC-4024	Organic Chemistry-I	3	1	4

Course Outcomes (COs)

- **CO1:** Explain the kinetics and energetics of organic reactions.
- **CO2:** Discuss reaction intermediates in organic reactions.
- **CO3:** Analyze the structure and reactivity of reaction intermediates in organic reactions.
- **CO4:** Classify the organic molecules on the basis their stereochemistry and compare their reactivity.
- **CO5:** Analyse and apply qualitative analysis techniques and separation of organic compounds using chromatographic techniques.

Theory (45 Hours)

Unit 1. Kinetics and Energetics of Reaction Mechanism (13 Hours)

- Transition state theory of reaction rates: kinetics & thermodynamics of activation. Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett principle; kinetic and thermodynamic control.
- Linear free energy relationships (LFER): Hammett equation- substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds; kinetic isotope effects in organic reactions.
- Effects of conformation on reactivity: anomeric effect, stereo electronic effects, neighbouring group participation.

Unit 2. Reaction Mechanisms & Intermediates: Structure & Reactivity I (12 Hours)

- Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination, Henry reaction, Nef reaction, Baylis-Hillman reaction.
- Ylids: Chemistry of phosphorous and sulphur ylids.
- Carbocation: structure and stability of carbocations, classical and non-classical carbocations, neighboring group participation and Wagner-Meerwein rearrangement.

Unit 3. Reaction Mechanisms &Intermediates: Structure & Reactivity II (10 Hours)

- Carbenes and Nitrenes: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition (existence of O and N based ylids), Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement, Tebbe olefination reactions.
- Radicals: Generation of radical intermediates and its addition to alkenes, alkynes (inter

& intramolecular) for C-C bond formation and Baldwin's rules.

Unit 4. Stereochemistry (10 Hours)

- Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; concept of absolute and relative configuration; chirality in molecules devoid of chiral centers - allenes, spiranes and biphenyls (atropisomerism).
- Concepts of stereogenic center-chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality); optical purity and enantiomeric excess; conformation of acyclic organic molecules, cyclohexane and decalins.

Laboratory (30 Hours)

1. Qualitative analysis: Binary mixture analysis (solid-solid/solid-liquid/liquid-liquid)
2. Chromatography experiments:
   (i) Qualitative TLC separation and identification
   (ii) Column chromatographic separation of a mixture of compounds.

Recommended Books

1. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. A. J. Kirby, Stereoelectronic Effects, 1st edition, OUP.
3. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry.
4. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd edition, OUP 2012.
5. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005
6. E.L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds.
7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.
8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
1	CHE-1-DSC-4034	Physical Chemistry-I	3	1	4

Course Outcomes (COs):

- **CO1:** Evaluate multicomponent chemical systems by analysing the knowledge of phase equilibria and spectroscopy.
- **CO2:** Examine the principles of chemistry using non-equilibrium and statistical thermodynamics.
- **CO3:** Create hands-on skill development on principles of thermodynamics, spectrophotometry using standard reactions inside laboratory.
- **CO4:** Investigate theoretical chemistry experiments by formulating molecular modelling and computational methods.
- **CO5:** Construct chemical information by selecting relevant experimental procedures and assembling results, considering accuracy, precision, limitations, and sources of error.

Theory (45 Hours)

Unit 1. Phase Equilibria and Non-equilibrium Thermodynamics (10 Hours)

- Gibbs phase rule and its application to three component systems – triangular plots-water-acetic acid–chloroform system, ammonium chloride-ammonium sulphate-water system
- Non-equilibrium thermodynamics: flux, forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects – Seebeck, Peltier and Thomson effect, BZ reaction.

Unit 2. Statistical Thermodynamics (18 Hours)

- Statistical mechanics of system independent particles: Ensembles, Maxwell Boltzmann, Bose-Einstein and Fermi Dirac Distributions, entropy and probability. Calculation of thermodynamic properties for independent particles, molecular partition functions- evaluation of translational, rotational, vibrational and nuclear partition functions.
- Thermodynamic properties of monatomic and diatomic gases (Sackur-Tetrode equation)- calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant.

Unit 3. Elementary Spectroscopy (14 Hours)

- Fundamental aspects of absorption and emission spectroscopy. Probability of transition, oscillator strength, dipole strength. Spontaneous and stimulated emission. Origin of selection rules using symmetry. Quantitative treatment of Fourier Transform spectroscopy.
- UV-visible spectroscopy: Electronic transitions, Franck-Condon principle, vertical transitions; Selection rules, parity, symmetry and spin selection rules.

Instrumentation. Application in organic structure analysis; polarization of transitions

- Fluorescence and phosphorescence spectroscopy: Jablonski Diagram, origin of fluorescence and phosphorescence processes, quantum yield, fluorescence quenching-static and dynamic. Instrumentation and applications.

Unit 4. Data Analysis (3 Hours)

- Linear Regression and Curve Fitting Techniques

Laboratory (30 Hours): (Minimum of 6 and at least two from each section)

A. **On Spectroscopy**:

1. Determination of the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
2. Determination of the composition of iron-salicylic acid complex spectrophotometrically by Job's method of continuous variation.
3. Investigation of the complex ion formation between $Ni^{2+}$and o-phenanthroline by Job's method.
4. Verify the mixture law of refraction and draw the calibration curve for mixtures like glycerol water, n-heptane/n-hexane and hence determine the composition of an unknown mixture of two components.
5. Calorimetric investigation of the reaction between acetone and iodine.
6. Calorimetric determination of the enthalpy of a solution of NH_4Cl from heat capacity.
7. Study of the complex formation between Cu^{2+} ion and ammonia by distribution method and find the composition of the complex.

*Other experiments on spectroscopy can be introduced from time to time

B. **On Thermodynamics**

1. Adsorption of dye on activated carbon and analysis of result by different adsorption models.
2. Determination of adsorption kinetics of dye on activated carbon or other adsorbents and estimate the free energy.
3. Determination of thermodynamic quantities ΔH, ΔS and ΔG of dye adsorption on activated carbon.
4. Simulation of real gas using any programming language/computer interface and evaluating the free energy.
5. Determination of the composition of an unknown mixture of two/three components and create a phase diagram.

6. Determination of the equilibrium constant and free energy of the reaction: $KI+I_2 \leftrightharpoons KI_3$ by distribution method.
7. Determination of the molecular surface energy and the association factor for ethyl alcohol.

   * Other experiments on phase equilibria/thermodynamics can be introduced as per convenience.

Recommended Books

1. P. Atkins, J. Paula, Physical Chemistry, 12^{th} Edition, Oxford University Press, Oxford 2022.
2. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, Viva Student Edition, 1^{st} Edition, 2011.
3. R.S. Berry, S.A. Rice and J. Ross, Physical Chemistry, 2^{nd} Edition, Oxford University Press, Oxford 2007.
4. D.A. McQuarrie, Statistical Mechanics, University Science Books, California, 2008.
5. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6^{th} Edition, Pearson, 2009.
6. R.S. Drago, Physical Methods in Chemistry, 1992
7. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002
8. J.R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3^{rd} Edition, 2006
9. Banwell and McCash, Fundamentals of Molecular Spectroscopy, 4^{th} Edition, McGraw Hill, 2017
10. J.B.Y adav, Advanced Practical Physical Chemistry, Goel Publishing House, 27^{th} Edition, 2008.
11. J.N. Gurtu and A. Gurtu, Advanced Physical Chemistry Experiments, Pragati Prakashan, 6^{th} Edition, 2014.
12. M. Halperin, Experimental Physical Chemistry, 2^{nd} Edition, Prentice Hall, Upper Saddle River, NJ07458
13. Other Sources: *Journal of Chemical Education*, ACS Publications

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
1	CHE-1-DSE-4044 (A)	Quantum Chemistry	3	1	4

Course Outcomes (COs)

- **CO 1:** Apply Dirac notation, Hilbert spaces, and Hermitian operators to calculate quantum states and expectation values.
- **CO 2:** Solve the Schrödinger equation exactly for particles in a ring, rigid rotors, and harmonic oscillators.
- **CO 3:** Determine wave functions and electronic structures for the H-atom, H_2 molecule, and benzene.
- **CO 4:** Use Hückel and Extended Hückel molecular orbital theories to analyze unsaturated carbon systems.
- **CO 5:** Apply perturbation and variation theories to evaluate stable and time-dependent two-level systems.
- **CO 6:** Analyze multi-electron atoms using the Born-Oppenheimer approximation, Pauli principle, and angular momentum coupling schemes.

Theory (45 Hours)

Unit 1. Wavepackets and Operators (8 h)

- Eigen values and Eigen vectors, Dirac bra-ket notation, review of vectors and vector spaces, Hilbert space
- Wave equation and interpretation in quantum mechanics, separation of time and space variables of the Schrodinger equation, Hermitian operators, matrix elements, The diagonalization of the Hamiltonian, wave-packets, wave functions of one particle and many particles system.
- Born interpretation, expectation values of observable properties.

Unit 2. Solution of Eigenvalue Equations (14 h)

- Solutions of the energy eigenvalue equations for particles in a ring, Rigid Rotor, Angular momentum operators, Step-up and Step-down operators, QM treatment of H-atom and H_2^+ molecule, Wave function of simple atomic and molecular orbitals.
- QM treatment of Harmonic Oscillator, Ladder operators. Free electron MO theory of benzene.

Unit 3. Approximate Methods (13 h)

- HMO treatment for unsaturated carbon compounds, extended Hückel Theory, elements of band theory.
- Time-independent perturbation theory of a two-level system (up to second order), the first order correction to the energy and wave function, perturbation theory for degenerate states, the second

order correction to the energy, time dependent behaviour of a two-level system, the Rabi formula, the effect of a slowly switched constant perturbation, the variation theorem, linear variation function-secular equation, the Rayleigh ratio.

Unit 4. Advanced Quantum Mechanics in Atomic Systems (10 h)

- Born-Oppenheimer approximation, product wave-functions, complete many electron wave functions including electron spin, Pauli's anti-symmetry and exclusion principles, Singlet and triplet states, central field model of many electron atoms (He atom), Slater type orbitals, splitting of term energies in presence of electric and magnetic field (Stark effect and Zeeman effect), L-S and J-J coupling.

Laboratory (30 Hours):

1. Use ball-and-stick models to visualize molecular structures and discuss concepts like bond lengths, angles, and molecular geometry.
2. Using computational software, analyze the molecular orbitals of various molecules to understand their electronic structure and bonding.
3. Least squares fitting and plotting linear and exponential graphs using computer.
4. Plotting the wave function and the energy expressions for particle in a box for n=1,2 and 3 using any spreadsheet software such as MSExcel/Libre Office etc or simple programming language.
   (GWBasic/ FORTRAN/ python etc).
5. Plotting simple one-dimensional intermolecular potential energies (e.g. harmonic, anharmonic, Lennard-Jones potential etc) using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GW Basic, FORTRAN, python etc) and provide necessary interpretation.
6. Geometry optimization (energy minimization) any polyatomic molecules: Making input file through selection of simple calculation method (e.g., Hartree Fock or Density Functional Theory), STO/GTO, basis set using any quantum chemistry software.
7. Perform geometry optimizations (energy minimizations) to calculate the energy of various conformations of molecules (e. g. butane) and predict the most stable conformation.

Recommended Books

1. P. Atkins, R. Friedman, Molecular quantum Mechanics, 4th Edition, Oxford University Press, Oxford 2008.
2. I. N. Levine, Quantum Chemistry, 7th Edition, PHI Learning Pvt. Ltd., 2014.
3. David J. Griffiths, Introduction to Quantum mechanics, 2nd edition, Pearson Education Ltd., 2014
4. A. Szaboo, N. S. Ostlund, Modern Quantum Chemistry, 1st edition (Revised), 2015.
5. Quantum Chemistry by Donald A McQuarrie

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
1	CHE-1-DSE-4044 (B)	Polymer Chemistry	3	1	4

- **CO 1:** Classify polymers, explain their nomenclature, structural texture, and the critical role of functionality in synthetic macromolecular formation.
- **CO 2:** Analyze the glass transition temperature () using free volume theory and the WLF equation, and evaluate the factors influencing it.
- **CO 3:** Formulate the mechanisms and kinetics of step-growth, chain-growth (radical, ionic, coordination), and co-polymerization techniques.
- **CO 4:** Determine polymer molecular weights, polydispersity index, and crystalline properties (morphology and melting point) using standard experimental methods.
- **CO 5:** Apply thermodynamic principles, including the Flory-Huggins theory and solubility parameters, to explain polymer solution behavior and phase stability (LCST/UCST).
- **CO 6:** Evaluate the preparation, structure-property relationships, and applications of commercial plastics, elastomers, thermosets, and advanced conducting polymers.

Theory: 45 Hours

Unit 1: Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Unit 2: Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems. Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

Unit 3: Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Unit 4: Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Unit 5: Determination of molecular weight of polymers

Determination of molecular weight of polymers (Mn, Mw, etc.) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

Unit 6: Polymer Solution:

Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures

Unit 7: Properties of Polymers (Physical, thermal, Flow & Mechanical Properties):

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

Laboratory (30 Hours):

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) /Methyl Acrylate (MA) / Acrylic acid (AA).
    a. Purification of monomer
    b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutylonitrile (AIBN)
2. Preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
    a. Preparation of IPC
    b. Purification of IPC
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin 6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).
8. Determination of molecular weight by viscometry:
    (a) Polyacrylamide-aq.NaNO2 solution
    (b) (Poly vinyl proplylidine (PVP) in water
9. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
10. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

11. Testing of mechanical properties of polymers.
12. Determination of hydroxyl number of a polymer using colorimetric method. Polymer analysis
13. Estimation of the amount of HCHO in the given solution by sodium sulphite method
14. Instrumental Techniques
15. IR studies of polymers
16. DSC analysis of polymers
17. Preparation of polyacrylamide and its electrophoresis

Text Books/References:

1. Stevens, M. P. (1999). *Polymer Chemistry: An Introduction* (3rd ed.). Oxford University Press. *(Note: The 3rd edition was originally published in 1999, though it has seen various reissues/reprints).*
2. Allcock, H. R., Lampe, F. W., & Mark, J. E. (2003). *Contemporary Polymer Chemistry* (3rd ed.). Prentice-Hall.
3. Billmeyer, F. W. (1984). *Textbook of Polymer Science* (3rd ed.). Wiley-Interscience.
4. Fried, J. R. (2003). *Polymer Science and Technology* (2nd ed.). Prentice-Hall.
5. Munk, P., & Aminabhavi, T. M. (2002). *Introduction to Macromolecular Science* (2nd ed.). John Wiley & Sons.
6. Sperling, L. H. (2005). *Introduction to Physical Polymer Science* (4th ed.). John Wiley & Sons.
7. Carraher, C. E., Jr. (2013). *Seymour/Carraher's Polymer Chemistry* (9th ed.). CRC Press / Taylor & Francis.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-DSC-5014	Inorganic Chemistry-II	3	1	4

Course Outcomes (COs)

- **CO1:** Assess the chemistry of main group elements.
- **CO2:** Summarize the structure, bonding and reactivity of heavy transition metals.
- **CO3:** Explain the structure, bonding and properties of solid-state materials.
- **CO4:** Analyze the structure, bonding and reactivity of organometallic compounds.
- **CO5:** Evaluate the mechanisms of inorganic reactions.

Theory (45 Hours):

Unit 1. Descriptive Inorganic Chemistry (16 Hours)

- Structure and bonding in polyhedral boranes and carboranes, electron count in polyhedral boranes – styx numbering, Wade's rules – polyhedral skeletal electron pair theory (PSEPT); Synthesis of polyhedral boranes. The hydroboration reaction, organoboranes, tetrahydridoborates – synthesis and synthetic use.
- Compounds of Al, Ga, In and Tl.
- Fullerenes and fullerides; Silica, silicates, clays and zeolites.
- Compounds of Si, Ge, Sn and Pb.
- Phosphates and phosphazenes; sulfur-nitrogen compounds; metal-oxo compounds; metal chalcogenides.
- Organometallic compounds of Li, Be and Mg.
- Chemistry of the second and third transition series elements –general overview of compounds having the metals in their common oxidation states.
- Halide containing clusters of niobium and tantalum; polyoxometallates of Mo and W; quadruple and quintuple M-M bonded compounds.

Unit 2. Introduction to Solid State Chemistry (6 Hours)

- Structure of simple solids–metals, alloys and compounds; common structure types.
- Bonding in solids–free-electron and band theory of solids.
- Properties of solids– optical, magnetic and electrical properties of solids.

Unit 3. Organometallic Chemistry (15 Hours)

- Synthesis, structure, bonding and reactivity of mono and polynuclear metal carbonyls, substituted metal carbonyls. Vibrational spectra of metal carbonyls.
- Types of M-C bonds – Synthesis, structure and reactivity of metal alkyls, alkenes, alkynes, arene and carbene complexes; metallocenes.
- Fundamental organometallic reactions: oxidative addition, reductive elimination, insertion, β-hydride elimination.
- Catalysis-hydrogenation, hydroformylation, alkene polymerization, olefin metathesis, Suzuki coupling reaction.

Unit 4. Mechanism of Inorganic Reactions (8 Hours)

- Substitution in octahedral and square planar complexes: Conjugate base mechanism, racemisation, stereochemistry, electron transfer reactions - inner sphere and outer sphere mechanism, Marcus theory.

Laboratory (30 Hours):

1. Quantitative analysis (binary mixture, alloy, ore) - Ca-Mg ore, Cu-Zn alloy, Pb-Sn alloy, Ni in an alloy *etc.*
2. Isomerism in coordination compounds: conversion of chloropentammine cobalt(III) chloride to nitro and nitroso isomers; *cis*- and *trans*-dichloro bis(ethylenediamine)cobalt(III) chloride *etc.*
3. Preparation of polyoxometalates, *e.g.* tetrabutylammonium hexamolybdate(VI) and characterization.
4. Quantitative determination of components in food (Fe, Zn, I, Ca, *etc.*)

Recommended Books

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6thed. Wiley, **1999**.
2. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; Shriver & Atkins' Inorganic Chemistry, 5th ed. Oxford University Press, **2010**.
3. Fundamental Concepts of Inorganic Chemistry, Vols.1-7, by A. K. Das and M. Das, CBS Publishers and Distributors, **2015**.
4. L. Smart, E. Moore, Solid State Chemistry: An Introduction, 2ndEd. Nelson Thorns Ltd. **2004**.
5. A. R. West, Solid State Chemistry and Its Application, Wiley Student Edition, John Wiley & Sons. **1998**.
6. R. H. Crabtree, Organometallic Chemistry of the Transition Metals 2nd Ed., John Wiley, **1993**.
7. C. Elschenbroich, A. Salzer, Organometallics: A Concise Introduction, 2nd Ed. Wiley VCH, **1995**.
8. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edition, Pearson, **2009**.
9. G. Svehla, S. Mittal, Vogel's Qualitative Inorganic Analysis, Pearson Education, 7th Edition, **2013**.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-DSC-5024	Organic Chemistry-II	3	1	4

Course Outcomes (COs)

- **CO1:** Apply fundamental concepts of organic photochemistry.
- **CO2:** Evaluate the diverse reactions of carbonyl compounds and olefins in photochemistry.
- **CO3:** Analyze complex photochemical rearrangement reactions.
- **CO4:** Evaluate oxidation and reduction reactions in organic synthesis.
- **CO5:** Apply principles of pericyclic reactions to predict reactivity and stereochemistry.

Theory (45 Hours):

Unit 1. Organic Photochemistry (10 Hours)

- Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems, Paterno-Buchi reaction, Photochemistry of enones.
- Photochemistry of olefins – photostereomutation of cis-trans isomers, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision.
- Photo-rearrangement reactions, di-π-methane rearrangement, Photo-rearrangement of cyclohexadienones, Barton rearrangement; Singlet oxygen photochemistry.
- Photochemistry of aromatic compounds.

Unit 2. Oxidation Reactions (10 Hours)

- Metal based and non-metal-based oxidations (Cr, Mn, Ag, Os, Ru, Se), DMSO, hypervalent iodine and TEMPO based reagents.
- Epoxidation with peracids, Baeyer-Villiger oxidation, Prevost reaction and Woodward modification.
- Sharpless asymmetric epoxidation, Sharpless asymmetric dihydroxylation.

Unit 3. Reduction Reactions (10 Hours)

- Catalytic hydrogenation (Pd/Pt/Ni). Wilkinson catalyst, Noyori asymmetric hydrogenation.
- Metal based reductions using Li/Na in liquid ammonia, Birch reduction, McMurry reaction, dehalogenation and deoxygenations.
- Hydride transfer reagents from Group III and Group IV in reductions ($NaBH_4$ triacetoxyborohydride, Luche reduction, $LiAlH_4$, DIBAL-H, Trialkyl silanes and Trialkyl stannane, Meerwein-Pondorff-Verley reduction.
- Stereo/enantio selective reductions (Chiral Boranes).

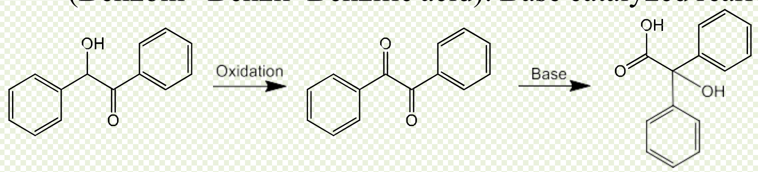
Unit 4. Pericyclic Reactions (15 Hours)

- MO symmetry, FMO of conjugated polyenes. Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry correlation method, PMO method.
- Cycloaddition reactions: 2+2, 4+2, 3+2 and 4+3 dipolar cycloadditions; stereoselectivity of the reactions, regioselectivity of 4+2 cycloaddition reaction.
- Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinyl cyclopropane rearrangement, fluxional molecules, stereo selectivity in Cope and Claisen rearrangement. Sommelet-Hauser rearrangement.
- Electrocyclic reactions and cyclo reversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.

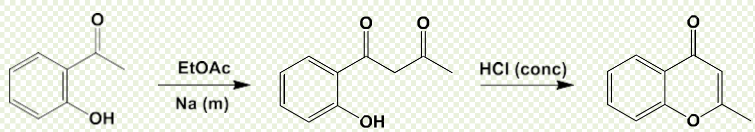
Laboratory (30 Hours)

1. **Synthesis (2-steps):**

- (Benzoin– Benzil–Benzilic acid): Base catalyzed rearrangement



- (2-Hydroxyacetophenone–1,3-diketone–Chromone): Acid catalyzed cyclisation



- Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazo-phenanthrene derivative.
- Conversion of phthalic anhydride to anthranilic acid via phthalimide.

2. **Quantitative analysis:**

- Estimation of amino acids using titrimetric methods.
- Estimation of sugars using titrimetric (redox) methods.
- Spectroscopic methods for estimation of functional groups.
- Estimating the formation/ stoichiometry of donor-acceptor complex involving anthracene and picric acid (Job's method).

- Chiral resolution of a racemic mixture by crystallization and determination of enantiomeric excess.

Books Recommended

1. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
2. M. B. Smith, Organic Synthesis, 2nd Edition, 2005.
3. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, First South Asian Edition 2005, Cambridge University Press.
4. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd edition, Oxford University Press 2012.
5. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2005.
6. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition, Harper & Row, 1987.
7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Text book of Practical Organic Chemistry, Pearson, 2012.
8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.
9. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition, Longman, 1978.
10. Selected articles from Journal of Chemical Education, ACS Publications.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-DSC-5034	Physical Chemistry-II	3	1	4

Course Outcomes (COs)

- **CO1:** Demonstrate the application of chemical kinetics principles
- **CO2:** Analyze molecular reaction dynamics
- **CO3:** Evaluate methods for studying fast reactions
- **CO4:** Critically assess theories of unimolecular reactions
- **CO5:** Apply principles of dynamic electrochemistry

Theory (45 Hours):

Unit 1. Chemical Kinetics (6 h)

- Oscillating reactions, chemical chaos, Belousov-Zhabotinski reaction, branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots.

Unit 2. Molecular Reaction Dynamics (6 h)

- The transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard sphere collision theory, kinetics of reactions in solution- diffusion controlled and chemically controlled reactions, TST of reactions in solution-Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Unit 3. Study of Fast Reactions (5 h)

- Stopped flow technique, temperature jump method, relaxation kinetics, linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Unit 4. Theories of Unimolecular Reactions (6 h)

- Theory of unimolecular reactions- Lindemann theory and its limitations, Hinshelwood modification, RRK theory, RRKM theory.

Unit 5. Dynamic Electrochemistry (7 h)

- Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions-structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions, Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions- derivation, validity and limitations, extended Debye-Huckel-Onsager equation. The random walk model of ionic diffusion-Einstein Smoluchowski reaction.

Unit 6. Theories of Electrical Interface (4 h)

- Electrocapillary phenomena- Lippmann equation, electron transfer at interfaces, polarizable and non-polarizable and nonpolaisable interfaces, Butler-Volmer equation, Tafel plot.

Unit 7. Electro-analytical Techniques (6 h)

- Voltametric techniques: cyclic voltammetry, differential pulse voltammetry (DPV), stripping voltammetry techniques
- Potentiometric techniques: ion selective electrodes and other applications
- Amperometric techniques: amperometric sensors and biosensors

Unit 8. Systems for Electro-chemical Energy Storage & Conversion (5 h)

- Batteries: Types of Batteries, Lead-acid batteries, Ni-Cd batteries and Li-ion batteries, Supercapacitors: Electrical double layer capacitor, Pseudo-capacitor, Fuel Cells

Laboratory (30 Hours)

1. Determination of the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using least squares calculation.
2. Study of the dynamics of an oscillatory reaction.
3. Study of the kinetics of reaction between iodine and acetone in acidic medium by half-life period method and determination of the order with respect to iodine and acetone.
4. Study of the decomposition kinetics of the formation of complex between sodium sulphide and sodium nitroprusside spectrophotometrically. Determination of the rate constant and order of the reaction.
5. Study of the kinetics of the reaction between peroxydisulphate and potassium iodide and to find the influence of ionic strength on the rate constant.
6. Study of the kinetics of oxidation of ethanol by chromium(VI) and to find the rate constant of the reaction. Also find the order of the reaction by half-life period method.
7. Study of the double exponential time dependence of the reduction of Cr(VI) by glutathione in an aqueous medium and to obtain the rate constants of the process.
8. Determination of the mechanism and rate constant for the oxidation of magnesium by hydrochloric acid.
9. Determination of the relative strength of two acids (HCl and H_2SO_4) by studying the hydrolysis of an ester (methylacetate/ ethyl acetate).
10. Investigation of the inversion of cane sugar in presence of HCl and H_2SO_4 and hence determination of the relative strengths of the two acids.
11. Investigation of the inversion of cane sugar in presence of acid and hence determination of the activation energy of the reaction.
12. Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence to find the degree of dissociation constant of the acid.
13. Comparison of the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
14. Determination of the degree of hydrolysis and hydrolysis constant of aniline

hydrochloride /sodium acetate.

15. Determination of the strength of the components of the following binary mixture by conductometric titration.
    - Hydrochloric acid and acetic acid
    - Sulphuric acid and copper sulphate
    - Hydrochloric acid and potassium chloride
    - nitric acid and sulphuric acid
16. Determination of the amount of each component of the following ternary mixture by conductometric titration. Hydrochloric acid, acetic acid and copper sulphate
17. Determination of the degree of hydrolysis and hydrolysis constant of CH_3COONa of NH_4Cl by conductance measurement.
18. Determination of the concentration of $AgNO_3$ by conductometric titration against KCl solution.
19. Cyclic voltammetry of a standard solution at different scan rates and calculation of redox potential of electro-active species.
20. Determination of diffusion coefficient from cyclic voltammetry.
21. Determination of Electrode surface area from cyclic voltammetry.
22. Determination of rate of heterogeneous electron transfer from cyclic voltammetry.
23. Chronocoulometry of a redox dye and determination of amount adsorbed on to the electrode surface.

(Students need to perform a minimum of six experiments: at least three from the chemical kinetics experiments and three from the rest)

Recommended Books

1. P. Atkins and J. Paula, Physical Chemistry, 9th Edition, Oxford University Press, Oxford 2010.
2. I. R. Levine, Physical chemistry, 6th Edition, Mcgraw Hill Education, 2011.
3. K. J. Laidler, Chemical Kinetics,3rd Edition, Pearson, 2012.
4. J. O. Bockris, A. K. N. Reddy, Modern Electrochemistry Part 1, 2A and 2B, 2nd Edition, Springer.
5. A. J. Bard, L. R. Faulkner, Electrochemical Methods Fundamentals and Applications, 2nd edition, Willy India, 2006.
6. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 27th Edition, 2008.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-DSE-5044(A)	Spectroscopy	3	1	4

Course Outcomes (COs):

- **CO1:** Explain the theoretical basis of different spectroscopic techniques.
- **CO2:** Analyse rotational, vibrational and Raman spectra, and data interpretation
- **CO3:** Demonstrable understanding of NMR spectroscopy principles, application of advanced NMR methods to examine dynamic processes.
- **CO4:** Apply the principles of EPR spectroscopy to study organic/inorganic compounds.
- **CO5:** Interpretation of mass spectra to deduce structure of biomolecules and organic/inorganic compounds.

Theory (45 Hours)

Unit 1. Rotational and Vibrational Spectroscopy (14 h)

- Rotational spectroscopy: Rotational spectroscopy of symmetric and asymmetric top molecules.
- Raman spectroscopy: polarizability tensor, Stokes and anti-Stokes lines, Origin of characteristic bands, instrumentation and applications in chemical and biological systems.
- Vibrational spectroscopy: Infrared and Raman spectroscopy of simple inorganic and organic molecules, Normal modes of vibrations, organic functional group identification using IR spectroscopy, analysis of representative spectra of metal complexes with various functional groups; application of isotopic substitution.

Unit 2. NMR Spectroscopy (17 h)

- NMR phenomenon, Zeeman splitting, factors affecting sensitivity and resolution of a NMR spectrum, chemical shift tensor, ^{1}H NMR-inductive and anisotropic effects on chemical shift (δ), chemical and magnetic equivalence.
- Second order effects in AB, AX and ABX spin systems, simplification of second order spectrum using high magnetic field. Application of ^{13}C NMR (DEPT) and δ ^{13}C to structural correlations, satellites.
- Pulse and Fourier transformation in NMR in various NMR experiments (1D DEPT and 2D COSY).
- Dynamic processes by VTNMR-restricted rotation (DMF, annulenes and related systems), ring inversion (cyclohexane), degenerate rearrangement (bullvalene) and fluxional inorganic molecules, fluxionality in organolithium compounds in solution. Derivation of activation energies and thermodynamic parameters from dynamic processes,
- NMR of Si, F, Xe, B, Li and P nuclei. NMR of paramagnetic metal complexes-contact and pseudo-contact shifts; magnetic moment measurement. Introduction to solid-state NMR-CP MAS.

Unit 3. EPR Spectroscopy (8 h)

- Electron Zeeman splitting, g-values, hyperfine and super-hyperfine coupling constants.
- EPR spectra of organic and inorganic radicals/compounds; zero field splitting, Kramer's degeneracy.

Unit 4. Mass Spectrometry (6 h)

- Mass spectrometry: basic principles and instrumentation, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation.
- ESI-MS and MALDI-MS-applications in biomolecules. Studies of inorganic/coordination and organometallic representative compounds.

Laboratory (30 Hours)

(Min. 6 experiments are to be performed from the following list of experiments)

1. Interpretation of infrared (IR) spectra of simple organic compounds. (The student is required to learn about identification of functional groups of simple organic compounds by interpreting the IR spectra. The spectra may be recorded and/or provided to the students from literature.)
2. Some representative examples are the following: Group A: cyclohexanol, cyelohexanone, cyclohexane etc. Group B: benzoic acid, salicylic acid, p-cresol etc. The student is required to identify unknowns from group A and B by the process of elimination)
3. Comparison of structural isomers for simple compounds using IR spectroscopy
4. Application of Nuclear Magnetic Resonance (NMR) Spectroscopy for the Characterisation of Small Molecules (e.g. Comparison of trans-2-hexenoic and trans-3-hexenoic acid spectra)
5. Interpretation of EPR spectrum of the simple molecules. (Students will be required to measure the value of g for DPPH and use it to determine the value of g for two inorganic complexes, $Cu(acac)_2$ and $VO(acac)_2$ etc. The spectra will be supplied to the students).
6. Density Functional Theory calculations of Normal Modes and Infrared intensities of simple molecule like water.
7. Structure elucidation of simple molecules using ^{1}H, ^{13}C NMR and mass spectrometry.
8. Interpretation of HR-MS spectrum of one simple organic molecule (The student is required to identify molecular ion peak and base peak; calculate the relative intensities and mass resolutions of all the peaks. The student is also required to propose a fragmentation pattern and explain why measured molecular mass is different from calculated mass. The data file will be supplied to the student).
9. Simulation of the proton NMR spectrum of an AX spin system from density matrices. (The student will be required to simulate the spectrum using density matrices by writing a script).
10. Calculation of chemical shifts of simple organic molecules using GIAO-based method using density functional theory.
11. Analysis of the reduction product of 3-nitrobenzaldehyde and similar

compounds using spectroscopic methods.

Recommended Books

1. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons, 4thEd.,2004.
2. D. L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 4th Ed., Cengage,2001.
3. R.S. Drago, Physical Methods in Chemistry, Thomson Learning, 1977.
4. R.M. Silverstein, F.X. Webster, D.J. Kiemle, D.L. Bryce, Spectrometric Identifications of Organic Compounds, 8th Edition, Wiley India Pvt. Ltd, 2015.
5. H. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 3rdEdn. Wiley-VCH, 2013.
6. W. Kemp, Organic Spectroscopy, 3rd Edition, Palgrave Macmillan, 2011.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-DSE-5044(B)	Petroleum Science and Technology	3	1	4

- **CO1:** Explain the origin, composition, and characteristics of crude oil fractions, and evaluate petroleum samples using standard assay parameters and product specifications.
- **CO2:** Analyze primary refinery operations, including fractionation, treatment techniques, asphalt technology, and catalytic pathways for light olefin production.
- **CO3:** Evaluate the fundamentals, kinetics, and catalytic advances in hydrotreating, hydrocracking, and fluid catalytic cracking (FCC) processes.
- **CO4:** Apply kinetics and integrated characterization methodologies to optimize deep desulfurization, dearomatization, and refinery product quality modelling.
- **CO5:** Categorize geochemical analytical methods for reservoir fluids and trace the production pathways of first, second, and third-generation petrochemicals.
- **CO6:** Appraise refinery pollution control strategies, emission standards (Euro/Bharat stage), and regulatory frameworks governing explosives and hazardous petroleum storage.

Theory: 45 Hours

Unit 1: Petroleum a Natural Resource: (8 Hours)

Origin (Theories of Organic and Inorganic Origin), Formation and Composition; Major petroleum fractions and products (refinery gases gasoline, naphtha, kerosene, diesel, fuel oil, lubricating oil); Hydrocarbons and non-hydrocarbons present (type, name, structure, role); Crude assay, evaluation of crude and petroleum fractions; Specification of petroleum products.

Unit 2: Petroleum Processing Overview: (10 Hours)

Petroleum processing data; Fractionation of petroleum; Treatment techniques; Thermal and catalytic processes practice in Petroleum refinery, Hydrotreating and Hydrocracking: Fundamentals; Recent advances in Hydrocracking; Current progresses in catalyst and catalysis of Hydrotreating; Asphalt Technology; Catalytic Processes for light Olefin production.

Unit 3: Modern Processing Techniques: (12 hours)

Kinetics and Mechanisms of Fluid catalytic cracking; Ultra deep Desulphurization of Diesel: How an understanding of the underlying kinetics can reduce Investment costs; Ultra-clean diesel fuels by Deep Desulphurization and Deep Dearomatization of middle distillates; Integrated methodology for characterization of Petroleum Samples and its application for Refinery product quality modeling.

Unit 4: Analytical and Separation Techniques: (10 Hours)

Quantitative and Qualitative Steps in Analysis of Petroleum; Analytical Methods in Geochemistry for Reservoir Rocks and Fluids; Distillation and Classification of Petroleum; First, Second and Third Generation Petrochemicals; Miscellaneous Petrochemicals.

Unit 5: Petrochemical Industry and Environment: (5 Hours)

Environmental pollution control in Petroleum refinery. Climate change and the petrochemical industry; Methodology and Assumptions for Estimating Particulate and Exhaust Emission; Euro and Bharat Stage emission limit; Petroleum rules, Gas cylinders rules-Explosives Act 1983.

Laboratory (30 hours):

1. Determination of the API Gravity and Specific Gravity of crude oil and petroleum products using hydrometers and pycnometers.
2. Determination of the Aniline Point of a petroleum fraction (diesel/kerosene) to estimate its aromatic content and hydrocarbon composition.
3. Determination of the Flash Point and Fire Point of lubricating oils and diesel fuel using the Pensky-Martens Closed Cup and Cleveland Open Cup apparatus.
4. Determination of the Kinematic Viscosity and Viscosity Index of lubricating oils at varying temperatures using a Redwood or Saybolt Viscometer.
5. Estimation of Smoke Point of kerosene and aviation turbine fuel (ATF) to assess burning quality and aromatic content.
6. Separation and qualitative identification of hydrocarbons (paraffins, olefins, aromatics) using Thin-Layer Chromatography (TLC) or standard chemical indicator methods (e.g., Bromine Number for olefins).
7. Determination of the Sulphur Content in diesel or gasoline via iodometric titration or turbidimetric methods to verify deep desulfurization efficiency.
8. Quantitative determination of the Acid Value/Total Acid Number (TAN) and Saponification Value of petroleum products to check for oxidative degradation and additives.
9. Field Study to nearest petroleum refinery

Text Books/References:

1. The Chemistry and Technology of Petroleum, James G Speight.
2. Advanced Petroleum Refining, G Sarkar, Khanna Publishers.
3. Modern Petroleum Refining Processes, B K Bhaskara Rao, Oxford and IBH Publishing Company Pvt Limited.
4. Chemicals from Petroleum by A. L. Waddams
5. Practical Advances in Petroleum Processing; Vol 1, Edited by C. S. Hsu and Paul R. Robinson, Springer.
6. Fundamentals of Petroleum Refining; Elsevier Limited.

7. Fundamentals of Industrial Catalytic processes, R. J. Farrauto, CH Bartholomew Blackie Academic & Professional, London 1997.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
2	CHE-2-FSC-5054	Analytical and Computational Chemistry	3	1	4

Course Outcome (COs):

- **CO-1 (Analyze):** Evaluate the reliability of analytical data using statistical tools, error analysis, and calibration methods.
- **CO-2 (Understand):** Explain the principles and instrumentation of advanced spectroscopic, chromatographic, and electrochemical techniques.
- **CO-3 (Apply):** Optimize molecular geometries and calculate molecular energies using computational methods like DFT and Ab Initio.
- **CO-4 (Predict):** Simulate and interpret thermodynamic properties and spectroscopic data (IR, NMR, UV-Vis) using quantum chemical modeling.
- **CO-5 (Synthesize):** Integrate experimental analytical data with computational models to solve complex chemical and structural problems.

Unit I: Purification and Separation Techniques (8 h)

Normal and reversed-phase liquid chromatography, partition, adsorption, ion-exchange chromatography; gas chromatography; and High-Performance Liquid Chromatography (HPLC). Hyphenated techniques, e.g., GC-MS and HPLC-ICP-MS.

Unit II: Electrochemical Methods of Analysis (7 h)

- **Polarography:** Linear scan polarography, Dropping Mercury Electrode (DME), and the Ilkovic equation.
- **Voltammetry:** Hydrodynamic voltammetry, amperometry, cyclic voltammetry, coulometry, and their applications.

Unit III: Thermal and Nuclear Methods of Analysis (10 h)

- **Thermal Methods of Analysis:** Thermogravimetry (TG), Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC): Principles, instrumentation, and applications.
- **Nuclear Methods of Analysis:** Neutron Activation Analysis (NAA) and X-ray Fluorescence (XRF) spectroscopy: Principles, instrumentation, and applications.
- **Atomic Absorption Spectroscopy (AAS):** Principles, instrumentation, methodology, and applications.

Unit IV: Introduction to Computers and Computing (10 h)

Introduction to basic computer tools (MS Word, PowerPoint, Excel). Spreadsheet (Excel)-based formula writing, basic mathematical operations, and graph plotting. Basic concepts of Python programming. Translation of spreadsheet-based calculations into simple Python programs.

Introductory awareness of the relationship between computer programming and AI/ML.

Unit V: Concepts in Computational Chemistry (10 h)
Scope of computational chemistry and its relation to molecular mechanics and quantum chemistry. Overview of empirical, semi-empirical, ab initio, and Density Functional Theory (DFT) methods (introduction to functionals and basis sets). Structure drawing, DFT-based geometry optimization, and frequency analysis using freely licensed software such as ORCA and Avogadro, and their relation to Potential Energy Surfaces (PES), local and global minima. Biomolecular visualization using VMD and Chimera.

Laboratory (30 Hours)

1. Thin-Layer Chromatography (TLC) of plant pigments using silica gel.
2. Separation of a binary mixture of metal ions using ion-exchange column chromatography.
3. Quantitative estimation of caffeine in beverages using Reversed-Phase HPLC.
4. Gas Chromatography (GC) analysis of volatile components in essential oils.
5. Identification of unknown organic compounds using pre-recorded GC-MS spectral libraries.
6. Determination of half-wave potential ($E_{1/2}$) of metal ions using polarography.
7. Cyclic Voltammetry (CV) study of the reversible ferricyanide/ferrocyanide redox couple.
8. Amperometric titration of lead ions with potassium dichromate.
9. Constant-current coulometric titration for the determination of bromine number in alkenes.
10. Thermogravimetric Analysis (TGA) of calcium oxalate monohydrate to monitor multi-step decomposition.
11. Differential Scanning Calorimetry (DSC) measurement of polymer glass transition (T_g) and melting (T_m) temperatures.
12. Quantitative determination of trace heavy metals in environmental water samples using Atomic Absorption Spectroscopy (AAS).
13. Qualitative elemental profiling of an alloy sample using X-ray Fluorescence (XRF) spectroscopy.
14. Spreadsheet-based linear regression plotting and equation solving ($y = mx + c$) for analytical calibration curves.
15. Writing a basic Python script using standard mathematical operations to automate common dilution calculations.
16. Importing a titration or chromatography CSV dataset to plot publication-quality graphs using Python's Matplotlib library.
17. Building a simple linear regression Machine Learning model in Python to predict a physical property from molecular weight.

18. Molecular structure drawing, bond metric measurements, and molecular mechanics geometry optimization using Avogadro.
19. Running a Density Functional Theory (DFT) geometry optimization and frequency analysis for a small molecule using ORCA to identify local minima.
20. Secondary structure rendering and active-site ligand distance measurements of a protein PDB file using VMD or UCSF Chimera.

Essential Reading

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West, and F.J. Holler, W.B. Saunders.
2. Analytical Chemistry: Principles, J.H. Kennedy, W.B. Saunders.
3. Analytical Chemistry: Principles and Techniques, L.G. Hargis, Prentice Hall.
4. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
5. Instrumental Methods of Chemical Analysis, B.K. Sharma, Goel Publishing House Ltd.
6. Essentials of Nuclear Chemistry, H.J. Arnikar, Wiley Eastern.
7. Quantum Chemistry, D.A. McQuarrie, University Science Books, Mill Valley, CA.
8. Molecular Quantum Mechanics, P.W. Atkins, Oxford University Press.

Additional Reading

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
3. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
4. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
5. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
6. Principles of Instrumental Analysis, D.A. Skoog and S.R. Crouch, W.B. Saunders.
7. Analytical Chemistry of Macroscopic and Supramolecular Compounds, S.M. Khopkar, Narosa, 2002.
8. Essentials of Computational Chemistry: Theories and Models, Christopher J. Cramer, 2nd Ed., Wiley & Sons, New York.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSC-5064	Foundations of Organic Synthesis and Green Chemistry	3	1	4

Course Outcomes (COs)

- **CO1:** Analyze dynamic stereochemistry in organic synthesis.
- **CO2:** Analyze retrosynthetic analysis principles and strategies.
- **CO3:** Evaluate the use of protecting groups in organic synthesis.
- **CO4:** Analyze the synthetic approaches and reactivities of heterocycles.
- **CO5:** Demonstrate synthesis of heterocyclic compounds and apply green synthesis techniques to organic compounds.

Theory (45 Hours)

Part A: Foundations of Organic Synthesis (30 Hours)

Unit 1. Dynamic stereochemistry (8 Hours)

- Stereospecific and stereoselective synthesis; classification of stereoselective synthesis, diastereoselective, enantioselective and double stereo-differentiating reactions, nucleophilic addition to aldehyde and acyclic ketones-Cram, Felkin and Felkin-Anh model, Prelog‘s rule, Stereoselective nucleophilic addition to cyclic ketones (Cram and Felkin-Anh models).

Unit 2. Retrosynthetic analysis (7 Hours)

- Basic principles of retrosynthesis, one group and two group C-C and C-X disconnections, amine and alkene synthesis, important functional group transposition and interconversions.

Unit 3. Protecting groups (5 Hours)

- Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection.

Unit 4. Introduction to heterocycles (10 Hours)

- Synthesis and reactivity of heterocycles containing one heteroatom (O, N, S) including furan, pyrrole, thiophene (Knorr, Paal-Knorr synthesis), pyridine (Hantzsch, Chichibabin synthesis), indole (Fischer, Bischler Synthesis), quinolone and isoquinoline (Combes, Conrad-Limpach, Skraup/Doebner-von Miller, Bischler-Napieralski, Pictet-Gams synthesis).

Part B: Green Chemistry (15 Hours)

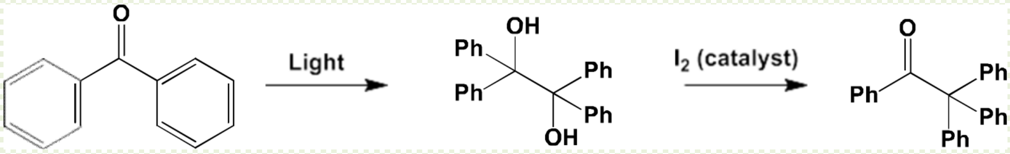
- Introductions to green chemistry and its principles (2 Hours)
- Catalysis and green chemistry- water oxidation, conversion of CO_2 utilizing CO_2 as a reactant (5 Hours)
- Renewable raw materials, utilization of renewable biomass, fuels and chemicals from biomass, concepts of platform molecules and conversion of biomass to value-added

products (5 Hours)

- Introduction to sustainability, aspects of sustainability ethics, designing sustainable solutions (3 Hours)

Laboratory (30 Hours)

1. Multicomponent reaction of aldehyde, β-keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction).
2. Multicomponent reaction of aldehyde, β-keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis).
3. Benzophenone - Benzopinacol - benzopinacolone): Photochemical, rearrangement.



4. Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using $NaBH_4$.
5. Synthesis of an aldol by reacting an aldehyde with a ketone.

Recommended Books

1. E. L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, Wiley, 2010.
2. F. A. Cary, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, McGraw Hill Higher Education, 2005.
4. W. Carruthers, I. Coldham, Modern methods of Organic Synthesis, Cambridge University Press, 2005.
5. J. J. Li, Name Reactions in Heterocyclic Chemistry, Wiley, 2006.
6. R. O. C. Norman, J. M. Coxon, Principles of Organic Synthesis, 3rd Edition, CRC Press.
7. M. Lancaster, Green Chemistry: An Introductory Text, RSC, 2002.
8. P. T. Anastas, J. C. Warner, Green Chemistry: Theory and Practice, Oxford University Press 2008.
9. J. H. Clark, F. Deswarte, Introduction to Chemicals from Biomass, 2nd Edition, Wiley 2015.
10. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.
11. Selected articles from *Journal of Chemical Education*, ACS.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSC-5074	Materials Chemistry	3	1	4

Course Outcomes (COs)

- **CO1:** Describe the fundamental principles of materials chemistry, including the classification of materials based on their chemical composition and structure.
- **CO2:** Apply knowledge of bonding interactions and crystal structures to predict material properties and behaviors in various solid-state systems.
- **CO3:** Synthesize and evaluate the correlation between material structure and properties, specifically in terms of mechanical, electrical, magnetic, optical, thermal, and surface characteristics.
- **CO4:** Analyze data obtained from various characterization techniques such as microscopy, spectroscopy, and diffraction of materials synthesized.
- **CO5:** Evaluate the potential applications of nanomaterials.

Theory (45 Hours)

Unit 1. Introduction to Materials (4 Hours)

- Overview of materials chemistry
- Classification of materials based on chemical composition and structure
- Nanomaterials

Unit 2. Solid state chemistry: (10 Hours)

- Bonding in materials: Ionic, covalent, metallic, and van der waals interactions.
- Crystal structure, crystal symmetry, crystal direction, crystal planes, defects in crystals and their impact on material properties,
- Reciprocal lattice, band structure, density of states and Fermi energy.
- Phenomena in low-dimensional systems- quantum confinement, quantum transport and surface plasmon resonance.

Unit 3: Properties of Materials (6 Hours)

- Structure property correlation Mechanical, Electrical, magnetic, Optical, Thermal and Surface properties of materials in bulk and nanomaterials.

Unit 4: Synthesis Methods (5 Hours)

- Solid-state synthesis techniques, Solution-based synthesis methods, Vapor-phase synthesis techniques, Hydrothermal and solvothermal methods, Nanomaterial synthesis: Bottom-up vs. top-down approaches.

Unit 5: Characterization Techniques (8 Hours)

- Optical microscopy and spectroscopy, Scanning electron microscopy (SEM) and transmission electron microscopy (TEM), X-ray diffraction (XRD) analysis, Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy, Thermal analysis techniques (DSC, TGA).

Unit 6: Fabrication Techniques (5 Hours)

- Chemical vapor deposition (CVD), Physical vapor deposition (PVD), Electrochemical deposition, Self-assembly and templating methods, Lithography techniques for nanofabrication

Unit 7: Applications (5 Hours)

- Nanoelectronics and nanophotonics, Nanomaterials in energy storage and conversion, Nanomedicine and drug delivery systems, Environmental applications of nanomaterials, Nanomaterials for sensing and diagnostics

Unit 8: Emerging Trends and Future Directions (2 Hours)

- Current trends in materials chemistry and nanomaterials research

Laboratory Experiments (30 Hours)

1. Synthesis of metal nanoparticles by chemical Reduction
2. Characterization of Carbon Nanotubes (CNTs) by Scanning Electron Microscopy (SEM).
3. Fabrication of Thin Film Solar Cells.
4. Preparation and Characterization of Quantum Dots.
5. Electrochemical Deposition of Metal Thin Films.
6. Synthesis of Graphene Oxide (GO) and Reduced Graphene Oxide (rGO).
7. Study of Surface Plasmon Resonance (SPR) in Metal Nanoparticles.
8. Fabrication of Polymer Nanocomposites.

Recommended Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver & Atkins‘ Inorganic Chemistry, 5th Ed., OUP
2. Bradley D. Fahlman. Materials Chemistry, Springer.
3. A. S. Edelstein; R. C. Cammarata. Nanomaterials: Synthesis, Properties and Applications. CRC Press
4. Charles P. Poole, Frank J. Owens, Introduction to Nanoscience and Nanotechnology. Wiley.
5. Edward L. Wolf. Nanophysics and Nanotechnology: An Introduction to Modern Concepts in Nanoscience. Wiley.
6. Geoffrey A. Ozin; André C. Arsenault. Nanochemistry: A Chemical Approach to Nanomaterials. Royal Society of Chemistry
7. Harry R. Allcock; Frederick W. Lampe; James E. Mark. Introduction to Materials Chemistry. Wiley.
8. A. R. West, Solid State Chemistry and its Applications, Wiley Student Edition, John Wiley & Sons.

9. R. Balasubramaniam, Callister's Materials Science and Engineering, 2nd Edition, Wiley.
10. M.S. Ramachandra Rao, S. Singh, Nanoscience and Nanotechnology: Fundamentals of Frontiers, Wiley India. 2016.
11. G. Schmid, Nanoparticles: From Theory to Application, Wiley-VCH Verlag.
12. G. Cao, Y. Wang, Nanostructures and Nanomaterials Synthesis, Properties, and Applications 2nd Ed. , World Scientific.
13. Gerrard Eddy Jai Poinern, A Laboratory Course in Nanoscience and Nanotechnology, CRC Press.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSC-5084	Surface Chemistry and Catalysis	3	1	4

Course Outcomes (COs)

- **CO1:** Proficiency in Catalyst Synthesis and Preparation.
- **CO2:** Demonstration of advanced proficiency in the principles and applications of homogeneous catalysis.
- **CO3:** Comprehension and application of the properties and functionalities of microporous and mesoporous materials.
- **CO4:** Proficiency in analysing the operation of catalytic reactors and identifying factors contributing to catalyst deactivation.
- **CO5:** Analysing Energy-Related Catalysis for insights.

Theory (45 Hours)

Unit 1. Catalysts synthesis and preparation (10 h)

Catalyst preparation methods – precipitation and co-precipitation – sol gel process–Dispersed metal catalysts; support materials; preparation and structure of supports; surface properties – preparation of catalysts –interaction of metal compound with substrate surface – metal distribution within catalyst pellets – metal cluster compounds as active precursors – pre-activation treatment – drying and calcinations – activation process. Bulk catalysts and supports. Heteropoly compounds – Solid superacids, carbon as catalyst support –carbon as catalyst.

Unit 2. Homogeneous Catalysis (10h)

Atom transfer and electron transfer processes, role of transition metal ions with special reference to Pd, Pt, Co, Ru, and Rh, catalysis in non-aqueous media, rate of homogenous catalytic reactions, turnover number and frequency, catalysis of isomerization, hydrogenation, oxidation and polymerization reactions, asymmetric catalysis, biocatalysis, photo- activated catalysis and metal clusters in catalysis, phase transfer catalysis.

Unit 3. Microporous and mesoporous materials (12 h)

Synthesis of aluminosilicate zeolites and related silica-based materials – structure, composition, synthesis of some selected important zeolites (titanosilicates), activation of zeolites. Modification of zeolites, ion exchange, metals supported on zeolites, dealumination and desilication of zeolites, Shape selective catalysis in zeolites. Mesoporous materials - ordered mesoporous materials –synthesis of silica molecular sieve materials -characterization of mesoporous molecular sieves – catalytic properties of mesoporous materials.

Unit 4. Catalytic reactors, deactivation of catalysts (8h)

Deactivation of catalysts – classification of catalyst deactivation processes; poisoning of catalysts (poisoning of metallic catalysts & poisoning of non-metallic catalysts, poisoning of bifunctional catalysts), metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts.

Design of catalytic reactors, Mass flow and heat flow minimisation.

Unit 5. Energy and catalysis (5h)

Energy related catalysis – Perspectives in oil refining – Steam reforming – Water gas shift– Methanol synthesis – CO and CO_2 hydrogenation, Catalytic reforming – Catalytic cracking, Hydrocracking, Catalytic converter, Fuel Cells.

Laboratory (30 h):

1. Analyzing the temperature coefficient and energy of activation in the acid-catalyzed hydrolysis of methyl acetate.
2. Study of the autocatalytic reaction between oxalic acid and $KMnO_4$ and determination of the order of the reaction.
3. Determination of the rate constants for the α-chymotrypsin-catalyzed hydrolysis of an ester.
4. Adsorption of dye on activated carbon and analysis of result by different adsorption models.
5. Study of the variation of surface tension of a solution of n-propyl alcohol/ethanol with concentration and determination of the limiting cross-sectional area of the alcohol molecule.
6. Exploring the base-catalyzed saponification of ethyl acetate with sodium hydroxide, with an aim to determine the reaction order and activation energy.

Recommended Books:

1. G. Ertl, H. Knozinger, J. Weitkamp (Eds), Preparation of Solid Catalysts, Wiley VCH Verlag, 1999.
2. J.R. Anderson, M. Boudart (Eds), Catalysis, Science and Technology, Vol 6, Springer-Verlag, 1984.
3. J. Weitkamp and L. Puppe (Eds), Catalysis and zeolites – fundamentals and applications, Springer-Verlag, 1999.
4. A. Gil, L.M. Gandia, M.A. Vincente, Catalysis Reviews Science and Engineering, 42 (2000) 145-212.
5. M. Hartmann, L. Kevan, Chemical Reviews, 99 (1999) 635-663.
6. A.B. Stiles, T.A. Koch, Catalyst manufacture, Marcel Dekker Inc., 1995.
7. R. Hughes, Deactivation of catalysts, Academic press, 1984.
8. G. Ertl, H. Knozinger, J. Weitkamp, Handbook of Heterogeneous Catalysis,Vol 4 and 5, Wiley-VCH, 1997.
9. R. J. Farrauto, C.H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Blackie Academic, Chapman and Hall, 1997.
10. R. Pearce, W.R. Patterson, Catalysis and Chemical processes, Academic press, 1981.
11. J. Weitkamp, L. Puppe (Eds), Catalysis and zeolites – fundamentals and applications, Springer-Verlag, 1999.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSE-5094	Advanced Bioinorganic Chemistry	3	1	4

Course Outcomes (COs)

- **CO1:** Explain active transport of ions and action potential in nerve impulses.
- **CO2:** Analyze the structural characteristics, functional roles, and catalytic mechanisms of diverse metalloenzymes.
- **CO3:** Evaluate the mechanisms of dioxygen reactions mediated by cytochrome *c* oxidase and oxygenase enzymes, and the role of detoxification enzymes in mitigating oxidative stress.
- **CO4:** Apply principles of electron transport and Marcus theory to analyze electron transport chains in biological system.
- **CO5:** Illustrate relevance of metal complexes in drug design with respect to metal-nucleic acid interactions, photodynamic therapy and diagnostic agents.

Theory (45 Hours)

Unit 1. Metal ion transport (4 Hours)

- Active ion transport across cell membrane, action potential (nerve impulse).

Unit 2. Metalloenzymes (8 Hours)

- Zinc enzymes: Useful characteristics of Zn(II) ion, Metal substitution in Zn enzymes -
- Carbonic anhydrase – structure, function, Co and Cu substitution studies, catalytic mechanism.
- Carboxypeptidase– structure of active site and catalytic mechanism.
- NiFe-hydrogenase, V-peroxidase.

Unit 3. Chemistry of dioxygen (15 Hours)

- Review of NMR and EPR in bioinorganic systems.
- Thermodynamics and kinetics of O_2 reactions -
- Cytochrome *c* oxidase: Spectroscopic characterization and mechanism of dioxygen reduction to H_2O.
- Dioxygenase: Spectroscopic characterization, mechanism and model complex study.
- Monooxygenase: Cytochrome P450 - structure, mechanism, porphyrin based model systems.
- Oxidative stress due to iron and copper *via* Fenton mechanism and

its consequences in human diseases; Detoxification enzymes - Catalases, Peroxidases and Superoxide dismutase.

Unit 4. Electron transport systems (8 Hours)

- Iron-Sulfur proteins, Cytochromes, Plastocyanine.
- Electronic coupling matrix, Marcus theory.
- Electron transfer chains– Energy storage and release: Aerobic respiration and photosynthesis; water splitting.

Unit 5. Metal-Nucleic acid interaction (7 Hours)

- Various types of interactions of metal complexes with DNA– coordination, intercalation, insertion, electrostatic and H-bonding and monitoring techniques.
- Applications of metal complex nucleic acid interactions; Interactions of *cis*-platin with DNA–evidence, kinetics, crosslinking reactions, biological consequences.
- Photodynamic therapy - photocleavage of DNA by transition metal complexes and its therapeutic implications.

Unit 6. Metals in clinical radiology (3 Hours)

- Gd-based MRI contrast agents, ^{99m}Tc and $BaSO_4$ (X-ray contrast agents).

Laboratory (30 Hours)

1. Synthesis and characterization of active site mimics of metalloenzymes:
   (a) zinc enzyme
   (b) catalase, peroxidase
   (c) superoxide dismutase
   (d) oxygenase
   (e) vanadium haloperoxidase, *etc.*
2. Assessment of interaction of metal complexes with DNA (drug-DNA interaction)-
   (a) Determination of intrinsic binding constants (K_b) of metal complexes having flat planar ligands such as phenanthroline bases with calf-thymus (CT)-DNA by UV-visible spectroscopic method.
   (b) Determination of apparent binding constants (K_{app}) of metal complexes by competitive fluorescent displacement method using ethidium bromide.
   (c) Determination of binding affinity of metal complexes with DNA by viscosity measurement.
   (d) Determination of binding affinity of metal complexes with DNA by thermal denaturation method.
3. Assessment of binding affinity of metal complexes with proteins (drug-protein interaction) such as serum albumins (HSA/BSA) by fluorescence

quenching method.

4. Assessment of ROS generation (hydroxyl radical, singlet oxygen etc.) abilities of metal complexes spectroscopically (absorption/emission) using chemical probes.
5. Synthesis and characterization MRI contrast agents and their applications.

Recommended Books:

1. Bioinorganic Chemistry by Bertini, Gray, Lippard, Valentine, Viva Books Pvt. Ltd., **1998**.
2. Bioinorganic Chemistry: A Short Course by R. M. Roat-Malone, Wiley Inter science
3. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life by W. Kaim, B. Schwederski, A. Klein, Wiley 2nd Ed. 2013.
4. Biocoordination Chemistry, D. E. Fenton, Oxford University Press.
5. Biological Inorganic Chemistry: An Introduction, R. R. Crichton, Elsevier.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSC-5104(A)	Supramolecular Chemistry	3	1	4

Course Outcomes (COs)

- **CO1:** Describe non-covalent interactions and the concept of pre-organisation in supramolecular chemistry
- **CO2:** Apply knowledge of various supramolecular structures (e.g., crown ethers, cyclodextrins) to understand their applications in molecular recognition.
- **CO3:** Analyze the design, synthesis, and applications of self-assembled structures like metallomacrocycles, MOFs, catenanes, and rotaxanes.
- **CO4:** Evaluate the relevance of supramolecular chemistry in mimicking biological systems, such as using cyclodextrins as enzyme mimics and ion channel mimics.
- **CO5:** Design molecular and supramolecular devices for specific functions, such as photonic devices, electronic devices, and molecular machines.

Theory (45 Hours)

Unit 1. Introduction to Supramolecular Chemistry (7 h)

Definition of supramolecular chemistry, biological inspiration for supramolecular chemistry, non-covalent interactions, host-guest interactions, pre-organisation: kinetic and dynamic effects, and complementarity, lock and key analogy.

Unit 2. Synthesis, structure and their applications in recognitions (12 h)

Crown ethers, podands, lariat ethers, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands binding of organic and inorganic cationic, anionic, ion pair and neutral guest molecules with host molecules, Supramolecular chiral recognition, ion-transport in biological system.

Unit 3. Self-Assembly of molecules (8h)

Design, synthesis and applications of metallomacrocycles, coordination polymers like metal organic frameworks (MOFs), catenanes, rotaxanes, helicates and knots, biochemical self-assembly, surfactants, micelles and vesicles, supramolecular liquid crystals.

Unit 4. Supramolecular Catalysis (8 h)

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, corands as ATPase Mimics, abiotic supramolecular catalysis.

Unit 5. Molecular Devices (10h)

Concept of molecular devices, molecular and supramolecular photonic devices, light conversion and energy transfer devices, molecular and supramolecular electronic devices, molecular wires, rectifiers, molecular switches (photo, electro, mechano etc.), molecular machines (gear, break, paddle wheel, shuttle etc.), molecular and supramolecular electrochemical devices.

Laboratory (30 Hours)

1. Determination of the CMC of a detergent by surface tension measurement.
2. Preparation and Characterization of a Triple Helicate Complex
3. Synthesis of molecular framework solids
4. Preparation of crown ethers
5. Application of crown ethers as phase transfer catalysts
6. Preparation of a monosubstituted cyclodextrin
7. Preparation of a rotaxane
8. Preparation of a C60-macrocyclic complex
9. Preparation of a Schiff base helicate component

Recommended Books

1. K. Ariga, T. Kunitake, Supramolecular Chemistry–Fundamentals and Applications, Springer, 2006.
2. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd Edition, John Wiley & Sons, 2009.
3. J-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley India Pvt. Ltd., 1995.
4. P. J. Cragg, A Practical Guide to Supramolecular Chemistry, John Wiley & Sons, 2005.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
3	CHE-3-DSE-5104(B)	Biochemistry	3	1	4

Course Outcomes (COs):

- **CO1:** Demonstrate understanding of cellular structure and function.
- **CO2:** Analyze bioenergetics and thermodynamics in living systems.
- **CO3:** Evaluate the chemistry of biomolecules.
- **CO4:** Analyze the role of metal ions in biological systems.
- **CO5:** Synthesize knowledge of biochemical principles and apply to real-world scenarios.

Theory (45 Hours)

Unit 1. Introduction (**5 Hours**)

- Prokaryotic and eukaryotic cells; structure of plant and animal cells; intracellular organelles and their functions; metabolic processes - catabolism and anabolism; constituents of cell nucleus, structure of chromosomes, cell division - mitosis and meiosis; composition and functions biological membranes -lipids and lipoproteins.

Unit 2. Biophysical chemistry (**10 Hours**)

- Bioenergetics- standard free energy change in biochemical reactions, ATP hydrolysis, synthesis of ATP from ADP; biological redox reactions, electron transfer and redox potentials of biologically important half reactions, oxidative phosphorylation.
- Thermodynamics of biopolymer solutions, osmotic pressure; active transport of ions through cell membrane; muscle contraction; energy generation in living systems; transmission of nerve impulses.

Unit 3. Bioorganic chemistry (**20 Hours**)

- Nucleic acid chemistry- structure and functions of DNA and RNA, the double helical structure of DNA; unusual DNA structure- DNA hairpins, triple helix, G-quadruplex; stability of the double helix-thermal denaturation and renaturation of DNA double helix; chemical and enzymatic hydrolysis of nucleic acids; DNA replication, RNA transcription and translation of genetic information.
- Carbohydrate metabolism- glycolysis, gluconeogenesis and Kreb's cycle.
- Biochemistry of lipids-biosynthesis of fatty acids, triglycerols, phospholipids, cholesterol and related steroids; prostaglandins.
- Protein biochemistry- amino acids, biosynthesis of amino acids, activation of amino acids, mechanism of translation, sequencing of amino acids in polypeptides; protein structure- primary, secondary tertiary and quaternary structure of proteins, post-translational modifications and protein folding.
- Enzymes- classification and catalytic behavior, enzyme kinetics, mechanism of action, factors affecting enzyme activity, enzyme regulators and inhibitors.

Unit 4. Bioinorganic chemistry (10 Hours)

- Role of metal ions in biology and their toxic effects; Iron management in biological systems –siderophores, ferritin and transferrin.
- Dioxygen storage and transport – structure of myoglobin and haemoglobin, cooperativity of O_2 binding in haemoglobin, Bohr effect and Hill coefficients.
- Electron transfer proteins (structure and function), Fe-S proteins, cytochromes and plastocyanines; structure of nitrogenase and its role in di-nitrogen fixation; structure and function of vitamin B_{12} and mechanism of 1,2-shift reaction; Inorganic therapeutics- chelate therapy, metal based drugs.

Laboratory (30 Hours)

Experiments on Natural products:

1. Introduction to extraction and phytochemical screening/ analysis of Natural Products (A case study).
2. Extraction of carotenoids from a natural source.
3. Isolation of (−)-Menthol from Peppermint Oil.
4. Saponification of Vegetable Oil.
5. Conversion of Vegetable Oil to Biodiesel.
6. Extraction of DNA from Onion peel.
7. Synthesis and characterization of therapeutically relevant metal complexes of first-row transition metals.

Books Recommended

1. D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry; 5^{th} edition, 2008 (W. H. Freeman & Co.).
2. R. H. Abeles, P. A. Frey, W.P. Jencks, Biochemistry, Jones and Bartlett Publishers, Boston, 1992.
3. D. Voet, J. G. Voet, C. W. Pratt, Fundamentals of Biochemistry: Life at the Molecular Level, 4^{th} Edition, 2012.
4. I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine, Bio-inorganic Chemistry; Viva books Pvt. Ltd.1998.
5. J. A. Cowan, Inorganic Biochemistry: An Introduction, 2^{nd} Edition, Wiley,1997.

Semester	Paper Code	Paper Title	Theory Credit	Practical Credit	Total Credit
4	CHE-4-PRJ-511-20	Dissertation	0	20	20

Course Outcome (COs):

- **CO 1:** Formulate Research Questions through Literature survey
- **CO 2:** Design and Execute Advanced Experimental Methodologies
- **CO 3:** Utilize Sophisticated Instrumentation and Structural Elucidation
- **CO 4:** Apply Critical Data Analysis and Deductive Reasoning
- **CO 5:** Uphold Research Integrity and Bioethics

The evaluation is divided into a 40% Continuous Internal Evaluation and a 60% End-Semester External Evaluation.

A. Continuous Internal Evaluation (CIE): 40 Marks

The internal assessment tracks regular progress, technical development, and lab ethics.

- **Supervisor Regular Assessment (15 Marks):** Evaluated by the research supervisor. Points are awarded for day-to-day bench regularity, adherence to laboratory safety/PPE protocols, technical handling of reagents, and maintenance of a verifiable, chronological Laboratory Research Notebook.
- **Mid-Term Review Seminar (15 Marks):** Evaluated by a departmental project review committee. The student presents a 15-minute slide detailing the literature foundation, clear research gaps, finalized *Aims & Objectives*, and preliminary optimization data.
- **Pre-Submission Presentation (10 Marks):** Presentation roughly 30 days before the final submission deadline. The student showcases their completed dataset, draft figures, and structural models to get clearance for binding the final thesis.

B. End-Semester External Evaluation: 60 Marks

The final grading is conducted by an appointed External Examiner from a university/colleges (having PG programme) or research institute. The evaluation is split into three core components:

Assessment Component	Weightage	Evaluated Parameters
Dissertation Report	**30 Marks**	Evaluation of structural organization, depth of literature review, clarity of experimental methodology, scientific discussion of results, and bibliographic accuracy (ACS/RSC/IUPAC style).
Final Project Presentation	**15 Marks**	Quality of visual data, defense of slides, time management, and the student's ability to clearly present complex chemical trends or reaction mechanisms.
Viva-Voce	**15 Marks**	Core domain knowledge, defense against technical critique by the external examiner, understanding of alternate mechanisms, and overall confidence.