# BODOLAND UNIVERSITY

## M.Sc. Syllabus in Chemistry under Choice Based Credit System (CBCS)
## (*w. e. f.* 2019–2020)

DEPARTMENT OF CHEMISTRY
Bodoland University
Kokrajhar – 783 370
Assam, India

**Department of Chemistry :: Bodoland University**

1. Name of the Course : **M.Sc. in Chemistry**
2. Duration of the Course : **Two Years (*Four Semesters*)**

**Semester–I**

| Course Code | Course Title | Credits (L+T+P) | Marks | | |
|---|---|---|---|---|---|
| | | | End-Sem | In-Sem | Total |
| CHM 101 | Physical Chemistry–I | 3+1+0=4 | 80 | 20 | 100 |
| CHM 102 | Organic Chemistry–I | 3+1+0=4 | 80 | 20 | 100 |
| CHM 103 | Inorganic Chemistry–I | 3+1+0=4 | 80 | 20 | 100 |
| CHM 104 | Spectroscopy–I | 3+1+0=4 | 80 | 20 | 100 |
| CHM 105 | Practical (Organic Chemistry) | 0+0+5=5 | 80 | 20 | 100 |
| CHM 106 | Open –I | 2+0+0=2 | 50 | 0 | 50 |
| | | **23** | | | **550** |

**Semester–II**

| | | | | | |
|---|---|---|---|---|---|
| CHM 201 | Physical Chemistry–II | 3+1+0=4 | 80 | 20 | 100 |
| CHM 202 | Organic Chemistry–II | 3+1+0=4 | 80 | 20 | 100 |
| CHM 203 | Inorganic Chemistry–II | 3+1+0=4 | 80 | 20 | 100 |
| CHM 204 | Spectroscopy–II | 3+1+0=4 | 80 | 20 | 100 |
| CHM 205 | Practical (Inorganic Chemistry) | 0+0+5=5 | 80 | 20 | 100 |
| CHM 206 | Open –II | 2+0+0=2 | 50 | 0 | 50 |
| | | **23** | | | **550** |

**Semester–III**

| | | | | | |
|---|---|---|---|---|---|
| CHM 301 | Quantum Chemistry | 3+1+0=4 | 80 | 20 | 100 |
| CHM 302 | Analytical Techniques | 3+1+0=4 | 80 | 20 | 100 |
| CHM 303 | Environmental Chemistry | 3+1+0=4 | 80 | 20 | 100 |
| CHM 304 | Advanced Topics in Chemistry | 3+1+0=4 | 80 | 20 | 100 |
| CHM 305 | Practical (Physical Chemistry) | 0+0+5=5 | 80 | 20 | 100 |
| CHM 306 | Elective–I | 3+0+0=3 | 80 | 20 | 100 |
| | | **24** | | | **600** |

**Semester–IV**

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|---|---|---|---|---|---|
| CHM 401/402/403/404/405/406 | Elective–II | 3+1+0=4 | 80 | 20 | 100 |
| CHM 401/402/403/404/405/406 | Elective–III | 3+1+0=4 | 80 | 20 | 100 |
| CHM 401/402/403/404/405/406 | Elective–IV | 3+1+0=4 | 80 | 20 | 100 |
| CHM 407/408/409 | Elective–V | 3+1+0=4 | 80 | 20 | 100 |
| CHM 410 | Project/Dissertation | 6 | 80 | 20 | 100 |
| | | **22** | | | **500** |
| | | **Total credits = 92** | | **Total marks = 2200** | |

**OPEN / ELECTIVE COURSES:**

| Course | | Course Title |
|---|---|---|
| **Open–I** | CHM 106-OP1 | Green Chemistry |
| | CHM 106-OP2 | Chemistry in Everyday Life |
| | CHM 106-OP3 | Basic Rubber Science |
| **Open–II** | CHM 206-OP1 | Renewable Energy |
| | CHM 206-OP2 | Petrochemical Process Technology |
| | CHM 206-OP3 | Polymer and Environment |
| **Elective–I** (***Any one paper***) | CHM 306-E1 | Biochemistry |
| | CHM 306-E2 | Computational Quantum Chemistry |
| | CHM 306-E3 | Solid State Chemistry |
| | CHM 306-E4 | Applied Electrochemistry |
| | CHM 306-E5 | Supramolecular Chemistry |
| **Elective–II, Elective–III & Elective–IV** (***Any three papers***) | CHM 401 | Polymer Science |
| | CHM 402 | Natural Products and Heterocyclic Chemistry |
| | CHM 403 | Transition Metals and Inorganic Materials |
| | CHM 404 | Catalysis |
| | CHM 405 | Organic Synthesis |
| | CHM 406 | Organometallics and Photoinorganic Chemistry |
| **Elective–V** (***Any one paper***) | CHM 407 | Chemistry of Surfactants |
| | CHM 408 | Bioorganic and Medicinal Chemistry |
| | CHM 409 | Bioinorganic Chemistry |

**Programme Specific Outcome (PSO)**

**PSO 1:** Acquire deep understanding to develop the problem solving skills using principles and processes of chemical sciences.
**PSO 2:** Develop skills of extraction, estimation, preparation, separation, and characterization of materials and chemical compounds following the chemical processes and using sophisticated analytical techniques.
**PSO 3:** Develop research and scientific writing skills through project/dissertation in the fields of chemistry such as organic, inorganic, physical, polymer science, analytical, etc.
**PSO 4:** Acquire knowledge in natural products, and biological and energy systems.
**PSO 5**: To well-equip the students with theoretical and analytical knowledge of different branches of chemical sciences to make them fit for industry jobs.
**PSO 6:** Theoretical knowledge gained through this course will help them to qualify national and international competitive examinations to fulfil their dreams as researcher/academician.

**Semester I**
**Course Code: CHM 101**
**Course Title: Physical Chemistry–I**
**Course Credit: 4**

*Course outcome*: Students will be able to understand the fundamentals of equilibrium and non-equilibrium thermodynamics, statistical mechanics, electrochemistry and polymers. With better understanding on these topics, their problem-solving capability will improve.

**Unit 1. Chemical Thermodynamics (16 h)**
Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions; Experimental determination of thermodynamic functions; Thermodynamic description of mixtures, Gibbs-Duhem equation; Chemical equilibrium; Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams; Thermodynamics of non-ideal systems– fugacity and activity concepts, excess properties.
Thermodynamics of real gases and gas mixtures, fugacity and its determination. Nonideal solutions, activity and activity coefficient- different scales of activity coefficients, electrolytic activity coefficients.
Thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to three-component systems- triangular plots- water-acetic acid chloroform and ammonium chloride-ammonium sulphate-water system.

**Unit 2. Non-equilibrium Thermodynamics (14 h)**
Difference between equilibrium and non-equilibrium thermodynamics, Criteria of nonequilibrium thermodynamics; uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces- relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; phenomenological relation: Onsagar relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

**Unit 3. Statistical Mechanics (12 h)**
Statistical mechanics of systems independent particles- Maxwell Boltzmann distribution, entropy and probability. Calculation of thermodynamic properties for independent particles-molecular partition functions - evaluation of translation, rotational, vibrational, electronic and nuclear partition functions. Thermodynamic properties of ideal monoatomic and diatomic gases (Suckur Tetrode equation)- calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant.

**Unit 4. Dynamic Electrochemistry (12 h)**
Ion-solvent interactions: 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-Húckel theory of ion-ion interactions – derivation, validity and limitations; extended Debye-Húckel-Onsager equation.

The random walk model of ionic diffusion - Einstein-Smoluchowski relation. Electro catalysis-influence of various parameters.

**Unit 5. Introduction to Polymers (10 h)**

Importance, historical background, raw materials and basic nature of polymers. Concept of monomer, repeating unit, degree of polymerization. Classification of polymers Average molecular weight concept. Polydipersity and molecular weight distribution. Measurement of molecular weights: end-group analysis, viscosity, light scattering, osmotic and ultracentrifugation methods.

**Semester I**
**Course Code: CHM 102**
**Course Title: Organic Chemistry–I**
**Course Credit: 4**

***Course outcome*:** Students will be able to demonstrate/explain the unique features of aromaticity, stereoelectronic factors, stereochemistry, organic reaction mechanism and reactivity & selectivity principles and will be able to solve related problems.

**Unit 1. Aromaticity and Stereoelectronic factors (10 h)**

Aromaticity and antiaromaticity– nonclassical concepts should be emphasized; HSAB concepts and their applications; symbiosis.

Stereoelectronic effects on reactivity– effect through bonds, through space; conformation and reactivity.

**Unit 2. Stereochemistry (20 h)**

Brief overview of the following: designation of configuration; Fischer-Sawhorse- Newman interconversion.

Molecular symmetry, asymmetry & dissymmetry; classification of organic molecules into different Point Groups; Concept of stereogenic center- chirotopic and achirotopic center; Homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality *etc*.); optical purity, determination of enantiomeric excess and diastereomeric excess; meaning of absolute and relative configuration; chirality in molecules devoid of chiral centers allenes, spiranes and biphenyls.

**Unit 3. Reaction Mechanism (18 h)**

Reaction intermediate *vs*. transition state, thermodynamic product *vs*. kinetic product; factors affecting mechanism and reactivity in nucleophilic substitution reactions; factors affecting mechanism and reactivity in elimination reactions, and competition with substitution reactions.

Kinetic & non-kinetic methods; kinetic isotope labeling studies; significance of rate limiting step in multi-step reactions; from rate law to mechanism and from mechanism to rate law. Hammett & Taft equation; partial rate factor.

**Unit 4. Reactivity & Selectivity principles (16 h)**
Reactivity- selectivity principle– chemoselectivity, regioselectivity, stereoselectivity & stereospecificity in substitution, elimination and addition reactions; steric acceleration and steric retardation.

**Semester I**
**Course Code: CHM 103**
**Course Title: Inorganic Chemistry–I**
**Course Credit: 4**

***Course outcome***: Students will be able to explain/critically examine the chemistry of chemical bonding, structure of solids and applications of redox chemistry.

**Unit 1. Chemical bonding (16 h)**
Chemical bonding of simple inorganic covalent compounds- molecular orbital treatments, hybridization; understanding molecular properties from bonding. Molecular orbital theory of homo- and heteronuclear diatomics, molecular orbitals of polyatomic molecules, molecular shape in terms of molecular orbitals- Walsh diagrams.
Atomic and ionic radii- bond length and bond strength, van der Waals forces. Hydrogen bonding interactions, effects of hydrogen bonding and other chemical forces on melting and boiling points and solubility.

**Unit 2. Structure of simple solids (16 h)**
Packing of spheres - hexagonal and cubic close-packing, tetrahedral and octahedral holes in close-packed structures - metals and alloys, solid solutions. The ionic model for the description of bonding in ionic solids. Characteristic structures of ionic solids - the NaCI and CsCI types, the sphalerite and wurtzite types of ZnS, the NiAs structure type, the perovskite and spinel structure types of mixed-metal oxides - importance of ionic radii and the radius ratios in determining structure type among ionic solids.Lattice energy considerations, thermal stability and solubility-of inorganic solids.

**Unit 3. Descriptive inorganic chemistry (12 h)**
Synthesis, structure, bonding and reactivity of boron hydrides including polyhedral boranes, carboranes and mettalocarboranes.
Allotropes of carbon (including fullerenes), phosphorous and sulfur. Chemistry of silicates, aluminosilicates, zeolite and clays.

**Unit 4. Acid-base (10 h)**
Hard and soft acid-base (HSAB) concept and its applications. Strength of oxo acids and halo acids, strength of inorganic bases, periodic trends in acidity and basicity of hydrides, oxides, oxyacids of non-transition elements: Relevance of acidity and basicity in catalysis.

**Unit 5. Redox Chemistry (10 h)**
Standard electrode potentials, $p^H$ dependence of electrode potentials. Redox stability of metal ions in water, oxidation by atmospheric oxygen. Applications of Latimer and Frost diagrams, redox behaviour of non-transition elements based on electrode potential data.

**Semester I**
**Paper Code: CHM 104**
**Paper Title: Spectroscopy–I**
**Course Credit: 4**

***Course outcome***: Students will be able to identify/elucidate the basis of different spectroscopic techniques, and demonstrate their various applications in analyzing and interpreting experimental data.

**Unit 1. Electronic spectroscopy (10 h)**

Electronic transitions, the Frank-Condon principle, ground and first excites states of diatomic molecules, selection rules on the basis of the symmetry properties of the electronic states. Vibronic transitions. Fluorescence and phosphorescence, laser action. Electronic spectra of conjugated, aromatic and coordination compounds - d-d and charge-transfer spectra. Change of molecular shape upon electronic excitation.

**Unit 2. Rotational (microwave) spectroscopy (16 h)**

(a) Classification of molecules according to their moments of inertia, rotational energy levels of HCl. Determination of molecular geometry by isotopic substitution effects on pure rotational spectrum. Stark effect, estimation of molecular dipole moments. Spectra of symmetric top and asymmetric top type molecules.

(b) Rotational Raman spectra - anisotropic polarizability. Specific selection rule in Raman spectroscopy, Stokes and anti-Stokes lines.

**Unit 3. Vibrational-rotational spectroscopy (16 h)**

(a) Diatomic molecules - force constants. Fundamental vibration frequencies. The anharmonicity of molecular vibrations and its effect on vibrational frequencies, second and high harmonics.

(b) Vibration-rotation spectrum of HCI - P, Q and R branches. Vibrational Raman spectra of diatomic molecules.

(c) Polyatomic molecules (*e.g.* $CO_2$, $NH_3$) - normal modes vibrations, symmetry of vibrations - group theoretical treatment. Elements of normal coordinate analysis for the $CO_2$ molecule.

**Unit 4. IR spectroscopy (10 h)**

IR spectroscopy – Characteristic bands for different functional groups, change in band frequency due to FGI. Effects of hydrogen bonding on band frequency. Problem solving.

**Unit 5. Nuclear Magnetic resonance spectroscopy and ESR (12 h)**

(a) Nuclear Magnetic Resonance Spectroscopy: Basic principles, origin of chemical shifts, factors affecting the chemical shifts and their interpretation, spin-spin coupling, relaxation processes. Proton and $^{13}C$ NMR spectroscopy of simple organic molecules, living systems–MRI. Introduction to the NMR of solids.

(b) Characteristics features of ESR spectra– line shapes and line widths. The g value and hyperfine coupling parameter (A)– origin of hyperfine interaction, contact and dipolar mechanisms. Spin Hamiltonian, anisotropy of g and A. ESR spectra of simple organic radicals, spectral behaviour transition metal complexes of octahedral and distorted octahedral geometry.

**Semester I**
**Course Code: CHM 105**
**Course Title: Practical (Organic Chemistry)**
**Course Credit: 5**

***Course outcome*:** Students will be able to perform qualitative and quantitative analysis of organic compounds and mixtures, and implement single-step and multi-step organic synthesis.

**A. Qualitative Organic Analysis (40 classes)**
Binary mixtures of organic compounds, covering compounds with major functional groups, should be given with an objective to train students in qualitative separation by physico-chemical methods and identifying the compounds by chemical analysis.

**B. Organic Estimation (8 classes)**

I. Glycine by sodium hydroxide in the presence of formaldehyde.
II. Number of hydroxy groups in a disaccharide by acetylation.
III. Percentage purity of carbonyl compounds by 2,4 dinitrophenylhydrazine.
IV. Carboxylic acid by Ag-salt method.
V. Glucose & sucrose in a mixture.

**C. Organic Preparation (12 classes)**

*One-step preparation*

I. Benzyhdrol from benzophenone by reduction in alkaline medium.
II. Anthraquinone from anthrancene by oxidation with chromium trioxide.

*Two-step preparation*

I. Benzanilide from benzophenone.
II. Benzilic acid from benzoin.
III. Dibenzyl from benzoin.
IV. Anthranilic acid from phthalic anhydride.

**D. Chromatographic Application (10 classes)**

I. Separation and identification of aromatic nitro compounds present in a binary mixture by TLC.
II. Separation and identification of amino acids present in a ternary mixture by paper chromatography.

**E. Experiments on Natural Products (10 classes)**

I. Soxhlet extraction of carotenoids/chlorophyll from carrot/tomato/papaya/ spinach and determination of $R_f$ values by TLC.
II. Isolation of nicotine from tobacco.
III. Extraction of milk proteins.
IV. Extraction of essential oils from orange peels/rose petals/clove/ginger.
V. Determination of Saponification / Iodine / Acid values of Vegetable Oil.

***N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.***

**Semester I**
**Course Code: CHM 106-OP1**
**Course Title: Green Chemistry**
**Course Credit: 2 (**32 h)

***Course outcome*:** Students will be able to explain and compare relationships between Green Chemistry and chemical laboratory and industry for the design of safer processes and chemicals.

1. The Essentials of Green Chemistry: Introduction to Interdisciplinary Study of Green Chemistry, Definition of Green Chemistry.
2. Applying the 12 Principles of Green Chemistry; Green Chemistry Metrics.
3. Waste: production, problems and prevention.
4. Catalysis and green chemistry; Green Chemistry and Sustainability; Green Chemistry to Health and Environment: Inherent Hazards, Challenges; Water oxidation; Conversion of $CO_2$, Utilising $CO_2$ as reactant.
5. Feedstock chemicals, Chemicals from Biomass, Concept of platform molecules. Conversion of biomass to value-added products.
6. Adverse Effects of Chemicals on Health and the Environment; Green Chemistry Problems.
7. Real World Solutions: Designing for Materials and Energy Efficiency; Designing for Degradation.
8. Introduction to Sustainability; Aspects of Sustainability Ethics; Designing Sustainable Solutions.

**Books Recommended**


1. M. Lancaster, Green Chemistry: An Introductory Text, RSC, 2002.
2. P.T. Anastas, J. C. Warner, Green Chemistry: Theory and Practice, Oxford University Press 2008.
3. J. H. Clark, F. Deswarte, Introduction to Chemicals from Biomass, 2nd Edition, Wiley 2015

**Semester I**
**Course Code: CHM 106-OP2**
**Course Title: Chemistry in Everyday Life**
**Course Credit: 2**

***Course outcome*:** Students will be able to understand and demonstrate the involvement of chemistry, chemical composition and chemical processes in the day to day social life.

**Unit 1 (10 h)**
Materials used in everyday life – metals, polymers, paper, cement, ceramics and glass, chemical products- petroleum products, petrochemicals and their use in day to day life, LPG; semiconductors, plastics, dyes, paints, fabric and clothing; medicines, soap and detergents, cosmetics and personal care products, fertilizer, pesticides, herbicides: their uses and toxicity.

**Unit 2 (12 h)**
Basic chemistry of medicine, food, nutrition, preservatives, drinking water, beverages, Negative aspects of chemistry and green chemistry: environmental pollution, carbon emission, industrial and vehicular pollution, water pollution, chemical mischief and adulteration, hazardous chemicals and chemical hazards, explosives, fireworks, disaster, green chemistry.

**Unit 3 (8 h)**
Chemistry in social life: green way of life at home, workplace; chemistry of love, esthetics, theatre and the arts, style and fashion, food habit.

**Text Book(s)**
1. Rao, C.N.R.; *Understanding Chemistry*, University Press (India) Ltd., Hyderabad, 1999.
2. Seager S.L. and Slabaugh, M.R. *Chemistry for Today–General, Organic and Biochemistry, 4th edn.*, (Brooks/Cole, 2000).

**Semester I**
**Course Code: CHM 106-OP3**
**Course Title: Basic Rubber Science**
**Course Credit: 2**

***Course outcome***: Students will learn the basic about Rubber: their origin, types and some of their applications.

**UNIT 1** (16 h)
Introduction of science of large molecule, various classifications of polymers. Basic concepts of rubber or elastomer.
Origin – natural rubber latex, tapping, processing, properties and applications.

Requirements for rubber elasticity, raw rubber, vulcanized rubber.
Characteristic properties of rubber/elastomer, glass transition temperature (Tg) and its influence on properties.

**UNIT 2** (16 h)
Brief introduction about compounding & processing, name of the machineries involved in compounding & processing and their roles.
Introduction of general purpose rubbers: Synthetic and Natural ex. NR, SBR, NBR and EPDM, their applications.

**Semester II**
**Course Code: CHM 201**
**Course Title: Physical Chemistry–II**
**Course Credit: 4**

***Course outcome***: Students will learn about the theoretical basis of various theories of chemical kinetics, reaction dynamics, catalysis, adsorption and surface chemistry and most importantly the ways/methods of validation of these theories.

**Unit 1. Basic Principles of Quantum Mechanics (16 h)**
Wave functions of one-particle and many-particle systems: Born interpretation. Well behaved functions and normalized functions. Schwartz inequality (without derivation).
Dynamical variables and quantum mechanical operators- Hermitian operators and their properties.
Eigenvalues and eigenfunctions of quantum mechanical operators, their physical significance. Schrodinger's wave equation. Orthogonal functions - Schmidt's orthogonalisation technique. Expectation values of observable properties. Compatible observables and compatibility theorem.
Incompatible observables and the (generalized) uncertainty principle from Schwartz inequality. Basic ideas about the theory of angular momenta– spin and orbital angular momenta, conservation of angular momenta. General angular momentum operators $J_x$, $J_y$, $J_z$, step-up and step-down operators. Eigenvalues of $J^2$ and $J_z$ operators. Coupling of orbital and spin angular momenta-theoretical basis of the L-S and j-j coupling schemes.

**Unit 2. Chemical Kinetics (12 h)**
Steady-state approximation and its applications. Oscillating reactions, chemical chaos. Belousov-Zhabotinski reaction. Straight-chain reaction- hydrogen-halogen reactions, alkane pyrolysis. Branching-chain reactions - the hydrogen oxygen reaction, explosion limits. Enzyme catalysed reactions, Michaelis-Menten mechanism - Lineweaver-Burk and Eadie plots, enzyme inhibition.

**Unit 3. Molecular Reaction Dynamics (12 h)**
Collisions of real molecules- trajectory calculations. Laser techniques, reactions in a molecular beam- reaction dynamics. Estimation of activation energy and the calculation of potential energy surfaces - the transition state theory (TST) of bimolecular gaseous reactions,

statistical and thermodynamic formulations. Comparison between TST and hard-sphere collision theory. Theory of unimolecular reactions - Lindemann theory and its limitations; 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 4. Homogeneous Catalysis (10 h)**
Atom transfer and electron transfer processes. Role of transition metal ions with special reference to Cu, Pd, Pt, Co, Ru and Rh, catalysis in non-aqueous media. Rates of homogeneously catalysed reactions, turnover number and frequency. Catalysis of isomerisation, hydrogenation, oxidation and polymerization reactions. Asymmetric catalysis, biocatalysis, photoactivated catalysis and metal clusters in catalysis. Phase-transfer catalysis.

**Unit 5. Adsorption and Surface Chemistry (14 h)**
Adsorption of gases on solid surfaces - Langmuir's theory and its limitations. Derivation of BET equation - determination of surface area of an adsorbent, thermodynamics of adsorption processes. Capillary condensation - adsorption in micropores, hysteresis loop. Kinetics of heterogeneous catalysis - Langmuir-Hinselwood model and Riedel-Eley model. Electrical aspects of surface chemistry, Electro kinetic phenomena, the structure of electrical double layer, Zeta potential and colloidal stability, Measurement of zeta potential. Surfactants – definition and classification, micelle formation and determination of critical micelle concentration. Reverse micelle and its application, solubilization, microemulsion.

## Semester II
## Course Code: CHM 202
## Course Title: Organic Chemistry–II
## Course Credit: 4

***Course outcome*:** After learning the course, students will acquire the detailed knowledge on stereoselective synthesis, oxidation and reduction reactions, pericyclic reactions and organic photochemistry.

**Unit 1. Stereoselective synthesis (10 h)**
Classification of stereoselective synthesis– diastereoselective, enantioselective & double stereodifferentiating reactions; nucleophilic addition to aldehyde and acyclic ketones- Cram, Felkin and Felkin-Anh model; nucleophilic addition to cyclic ketones.
Enantioselective synthesis– use of chiral reagent, chiral catalyst and chiral auxiliary.

**Unit 2. Oxidation reactions (16 h)**
Allylic oxidation of atkenes– use of chromium trioxide-pyridine complex (Collin's reagent) and selenium dioxide.
Oxidation of alcohols– use of PCC, PDC, Swern oxidation, Mn (IV) oxide, silver carbonate, tetrapropylammonium perruthenate (VII). Oxidation of 1,2-diols - use of periodic acid and Pbtetraacetate.
Oxidation of carbon-carbon double bonds– perhydroxylation by $KMnO_4$, $OsO_4$ (including Sharpless dihydroxylation & epoxidation), oxidation with iodine, silver carboxylate and

peroxy acids; introduction to electrooxidation– oxidation of tertiary amines, alkenes and carboxylates.

**Unit 3. Reduction reactions (14 h)**
Use of $H_2$/Pd-C, LAH, $NaBH_4$, $NaCNBH_3$, 9-BBN, Lindlar catalyst, DIBAL, diimide, alkali metals in liquid ammonia, super hydride and selectrides; chiral reducing agents; introduction to electroreduction- reduction of carbonyl compounds, alkyl halides and nitro compounds.

**Unit 4. Pericyclic reactions (16 h)**
Introduction of pericyclic reactions, MO symmetry; FMO of conjugated polyenes. Woodward- Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions. Cycloaddition reactions |2+2|, |4+2|, |6+2| cycloadditions, stereoselectivity of the reactions. Sigmatropic rearrangement- fluxional molecules, stereoselectivity in Cope and Claisen rearrangements.

**Unit 5. Organic Photochemistry (8 h)**
General principles of photochemistry; excited state and photosensitization, photochemical processes–chemiluminescence, chemical and photochemical method of producing singlet oxygen, photostereomutation of cis-trans isomers.

**Semester II**
**Course Code: CHM 203**
**Course Title: Inorganic Chemistry–II**
**Course Credit: 4**

***Course outcome***: Students will be able to apply their knowledge of inorganic and solid state chemistry in explaining, interpreting and critically examining bonding/structure/reactivity of metal complexes and lanthanides and actinides.

**Unit 1. Coordination Chemistry I (16 h)**
General properties of transition elements, coordination compounds - types of ligands and complexes. Mononuclear complexes - commonly observed coordination geometries and their symmetry properties. Tetragonal, rhombic and trigonal distortions in octahedral complexes.

**Unit 2. Coordination Chemistry II (16 h)**
Crystal field theory of bonding in octahedral, tetrahedral and square planar transition metal complexes. Factors affecting crystal field splitting, crystal field stabilization energy, spectrochemical series. Ligand field theory of metal complexes- electronic spectra– d-d spectra interpretation of spectral behaviour of octahedral and tetrahedral complexes. Charge transfer spectra.

**Unit 3. Complexes of π-acceptor ligands and organometallic chemistry (12 h)**
Synthesis, structure, bonding, and reactivity of transition - metal complexes of π–accepting ligands such as CO, NO, $PPh_3$. Metal carbonyl hydrides and metal carbonyl clusters. Metal -

metal bonding in $Re_2Cl_8^{2-}$. Complexes containing alkenes and alkynes as ligands- Ferrocene - synthesis, structure, bonding and reactivity.

**Unit 4. Reactivity of complexes (10 h)**
Stability constants, the chelate effect, labile and inert complexes, mechanism of substitutionreactions in octahedral complexes and associated stereochemical changes, isomerisation and racemisation of tris-chelate complexes. The trans effect. Electron transfer reactions - outer and inner sphere mechanism.

**Unit 5. Chemistry of lanthanides and actinides (10 h)**
Important aspects of the chemistry of the lanthanides - oxidation states, lanthanide contraction, separation of lanthanide elements, lanthanide shift reagents. Chemistry of actinides – electronic configurations, oxidation states, sources of the actinide elements, their extraction and application. Radioactivity of actinides.

**Semester II**
**Course Code: CHM 204**
**Course Title: Spectroscopy–II**
**Course Credit: 4**

***Course outcome*:** Students will be able to explain the basic working principle of various spectroscopic techniques and will be able to apply their knowledge in analytical purposes and interpretation of data.

**Unit 1. Mass spectroscopy (8 h)**
Mass spectroscopy– Ion fragmentation mechanism, base peak and molecular ion peak, nominal mass and exact mass, isotopic distribution–problem solving.

**Unit 2. NMR spectroscopy (16 h)**
Chemical shifts and splitting patterns of signals, coupling constant and its distinction from chemical shift - use of coupling constant in structural elucidation. Simplification of spectra by use of shift reagents and high magnetic fields, integration and its use in proton count and molecular ratios - determination of enantiomeric excess. Deuterium exchange technique in the determination of labile hydrogen, spin-decoupling and NOE, $^{13}C$ NMR (DEPT), Complexity of $^{13}C$ NMR spectra and use of spin decoupling in its simplificalion, CINDP and its applications. Worked out examples using application of NMR.

**Unit 3. Optical spectroscopy and chiroptical properties (8 h)**
UV-visible spectroscopy- $\lambda_{max}$ and molar absorptivity, factors affecting them. Calculation of $\lambda_{max}$ - Woodward Fieser's rules.
Chiroptical properties - introduction to CD (Circular Dichroism), ORD (Optical Rotatory Dispersion) and CPE. Applications of CD and ORD - octant rule.

**Unit 4. Vibrational and electronic spectroscopy (16 h)**

(a) Symmetry criteria for intensity of spectroscopic transitions (qualitative treatment), symmetry and spectral changes upon coordination. Infrared and Raman Spectroscopy: Symmetry and IR/Raman activity of normal modes of vibrations, Mutual exclusive principle, interpretation of IR and Raman spectra of simple inorganic and coordination compounds.

(b) Study of metal-ligand equilibria and Job's method, CD, ORD and MCD of inorganic compounds.

(c) Photoelectron spectroscopy: Basic principles and applications of PES ($O_2$, $N_2$ and $N_3^-$) only, chemical information from ESCA.

**Unit 5. ESR, NMR and Mossbauer spectroscopy (16 h)**

(a) ESR Spectroscopy: Basic principles, factors effecting g-tensors, hyperfine splitting in inorganic free radicals and metal complexes, zero field splitting. Applications of ESR to $d^1$ and $d^9$ complexes of various symmetry.

(b) NMR Spectroscopy: Simple application to diamagnetic inorganic compounds, NMR paramagnetic shifts, simple application to paramagnetic compounds. NMR of $^{31}P$ and $^{19}F$ in inorganic compounds.

(c) Mossbauer: Basic principles, isomer shift, quadruple splitting, and effect of magnetic field. Application to the study of high-spin and low-spin iron compounds and Sn compounds in various oxidation states and coordination geometries.

**Semester II**
**Course Code: CHM 205**
**Course Title: Practical (Inorganic Chemistry)**
**Course Credit: 5**

***Course outcome***: Students will be able to demonstrate experimental skills encompassing set-up of experiments, synthesis, characterization of different inorganic materials, and usage of analytical equipments.

**A. Qualitative and Quantitative Analysis (30 classes)**

(a) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe *etc.* involving volumetric and gravimetric methods.

(b) Analysis of ores/alloys, cement and steel, etc.
Ores: Hematite, Limestone, Dolomite, Cement, Pyrolusite, and other ores.
Alloys: Brass, Gunmetal, cupronickel, Solder, Bronze, Phosphor Bronze, Steel, Copper concentrate, other alloys.

(c) Determination of hardness of water.

**B. Preparation and characterization (50 classes)**

Preparation of selected inorganic compounds and their physicochemical characterization by elemental analysis, IR and electronic spectrophotometry, magnetic susceptibility measurements, magnetic resonance spectroscopy, solution conductivity measurements, wherever appropriate and possible.

(i) *Complexes with O-donor ligands*

(a) $A_3M(C_2O_4)_3$ –M = Al, Cr, Fe; A = alkali metal

(b) $VO(acac)_2$

(c) $Cu_2(OAc)_4(H_2O)_2$

(d) $Cu(acac)_2$

(ii) *Complexes with N donor ligands*

(a) $[Co(NH_3)_5Cl]Cl_2$, $[Co(NH_3)_5(ONO)]Cl_2$, $[Co(NH_3)_5(NO_2)]Cl_2$

(b) $Hg[Co(NCS)_4]$

(c) $Ni(dmg)_2$

(d) $NH_4[Cr(NH_3)_2(SCN)_4]$

***N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.***

**Semester II**
**Paper Code: CHM 206-OP1**
**Paper Title: Renewable Energy**
**Course Credit: 2**

***Course outcome*****:** After learning the course, students will acquire the detailed knowledge on renewable energy, conversion processes and applications.

**Unit 1 (16 h)**

Brief introduction to conventional energy and causes of energy scarcity. Introduction to renewable energy, sources and need and benefit of renewable energies. Energy scenario, economical aspects of renewable energy systems, sustainability issues.

**Unit 2 (16 h)**

Biomass energy and conversion processes, solar energy, geothermal energy, hydroelectric energy, wind energy, ocean energy, hydrogen gas as fuel. Energy storage systems. Concept of biorefinery and its importance.

**Semester II**
**Paper Code: CHM 206-OP2**
**Paper Title: Petrochemical Process Technology**
**Course Credit: 2**

***Course outcome*:** After learning the course, students will acquire the detailed knowledge on physicochemical properties petroleum products and their technological processes.

**Unit 1 (10 h)**
Petrochemical feedstock in India (Petroleum fractions, natural gas, tertiary recycling, pyrolysis gasoline); Petrochemical product profile (Polymers, synthetic fibre, synthetic rubber, detergent, intermediates).
Physico-chemical properties of hydrocarbons, crude oil evaluation, crude quality and pre-treatment of crude oils, natural gas processing, petroleum refining process, sulphur recovery, petroleum products.

**Unit 2 (10 h)**
Steam cracking for production of olefins, steam cracking process technology – Hot section, cracked gas compression & dehydration, operating variables in steam cracking, thermal cracking reactions, coke formation, decoking in thermal cracker, emerging technologies for olefins production.

**Unit 3 (12 h)**
Reactions in catalytic reforming, reforming catalysts, process variables in catalytic reforming, aromatic extraction & separation, dearomatizing of naphtha, aromatic conversion processes– disproportionation of toluene, hydroalkylation and isomerization. Synthesis gas and ammonia production, urea production, synthesis gas process technology, CO, Fischer-Tropsch Syngas technology, methanol, formaldehyde and acetic acid production. Ethylene and ethylene derivatives, propylene and its derivatives.

**Books Recommended**:

1. Petrochemical Process Technology by I. D. Mall

**Semester II**
**Paper Code: CHM 206-OP3**
**Paper Title: Polymer and Environment**
**Course Credit: 2**

***Course outcome***: Students will be able to know about the use of environmentally friendly polymers, their source, potential applications and management in minimizing their negative effect on environment.

**UNIT 1 (16 h)**

Synthetic polymers and their raw materials, fate of polymeric wastes & their impact on environment: Environmental problems caused by synthetic polymers.
Environmental biodegradability: Fate and Environmental effects.
Polymer degradation: Definition of biodegradable polymers, structural requirement for biodegradable polymers.

**UNIT 2 (16 h)**

Environmental Friendly Polymer: Polymers derived from natural sources, biopolymers, synthetic biodegradable polymers.
Recycled polymer: Methods of recycling, applications of recycled polymers. Plastic identification code.

**Semester III**
**Paper Code: CHM 301**
**Paper Title: Quantum Chemistry**
**Course Credit: 4**

***Course outcome***: Students will be able to know the several theories and methods of quantum chemistry and their successful applications in calculation of various theoretical parameters, e.g. energy etc.

**Unit 1. Approximate Methods of Quantum Mechanics (10 h)**

Time-independent first-order perturbation theory for (i) non-degenerate and (ii) degenerate systems; applications to the ground and first -excited states of the helium atom. The Variation theorem, linear variation function - Secular equation.

**Unit 2. Electronic Structure of Many-electron Atoms (12 h)**

Product wave functions - complete many-electron wave functions including electron spin. Pauli's Anti-symmetry and exclusjon principles. Spin states of a two-electron system - singlet and triplet states.
Independenl particle cetral field model of many-electron atoms- the helium atom. Atomic orbital theory- Slater type orbitals (STO), electron repulsion parameters (Racah and Condon-Shortley types).

Spectroscopic term symbols for the $s^1p^1$, $p^2$ and $d^2$ configurations - splitting of term energies due to electron repulsion and magnetic effects- spin-orbit coupling and Zeeman splitting.

**Unit 3. General Theorems in Molecular Quantum Mechanics (12 h)**

Born-Oppenheimer approximation, separation of electronic and nuclear motion. Hellmann-Feynmann theorem and its chemical applications. The electrostatic theorem and the force field concept in chemistry. Introduction to the molecular electronic Virial theorem. Elementary ideas about Density Functional Theory.

**Unit 4. Chemical Bonding (16 h)**

The hydrogen molecule ion: linear combination of atomic orbital (LCAO)-molecular orbital (MO) theory - ground and excited electronic states.
The hydrogen molecule: LCAO-MO and valence bond (VB) treatments. Equivalence of the MO and VB methods.
Extension of the LCAO-MO method to homo- and heteronuclear diatomics- inclusion of hybridizalion.
Term symbols for molecular electronic states, their symmetry classification- ligand field terms. Correlation diagrams and the non-crossing rule.
LCAO-MO theory of simple polyatomic molecules (e.g. $BeH_2$, $H_2O$ molecule).
Electron theory- Huckel molecular orbital (HMO) method for unsaturated carbon compounds showing chain and ring structures, introduction to extended Huckel theory. HMO treatment of infinite linear polyenes, elements of band theory.

**Unit 5. Ab initio and Semi-empirical SCF Theories (14 h)**

The self-consistent field method, Hartree-Fock theory of closed shell electronic configurations of atoms and molecules. Coulomb and exchange integrals, canonical Hartree-Fock equations, Koopman's theorem (without derivation).
SCF LCAO-MO theory of molecules - Roothan equation.
Semi-empirical SCF theory: Parriser–Parr-Pople approximation.

**Semester III**
**Paper Code: CHM 302**
**Paper Title: Analytical Techniques**
**Course Credit: 4**

***Course outcome***: Students will be able to explain/demonstrate the application of different analytical techniques in chemistry.

**Unit 1. Chromatographic methods (20 h)**

Adsorption, liquid-liquid partition, ion–exchange, paper and thin-layer chromatography, effect of solvent polarity on retention factor, reagents commonly used in the detection of TLC spots, HPLC, HPTLC, gel permeation chromatography, gas chromatography, flash chromatography, GC-MS and LC-MS.

**Unit 2. Electrochemical, Thermal and X-ray diffraction methods (20 h)**
(a) Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.
(b) Thermal methods: Principles and applications of thermogravimetry, DTA, TGA and DSC of inorganic compounds.
(c) X-ray methods: X-ray diffraction, X-ray fluorescence and X-ray absorption and X-ray emission spectroscopy.

**Unit 3. Microscopy (14 h)**
Scanning Electron Microscopy (SEM, FESEM), Transmission Electron Microscopy (TEM, HRTEM), Atomic Force Microscopy (AFM).

**Unit 4. Analysis of Metals (10 h)**
Preparation of sample for trace metal analysis in water, air, soil and plants, Extraction and dissolution techniques, Microwave digestion, Atomic absorption spectroscopy, Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy).

**Semester III**
**Paper Code: CHM 303**
**Paper Title: Environmental Chemistry**
**Course Credit: 4**

***Course outcome***: Students will be able to demonstrate an understanding of environmental chemistry viz. air, water and soil chemistry and identify the relationships between atmosphere, solar radiation and ozone formation.

**Unit 1. Environmental Chemistry: Global Perspective (10 h)**
Introduction to Environmental Chemistry, Chemical processes in the environment, Water cycle and its implications, Water resource flux, Case histories of environmental disasters and accidents.

**Unit 2. Atmospheric Chemistry (20 h)**
Temperature and pressure variations in the atmosphere, Chemical composition of the atmosphere and the influence of solar radiations, Thermodynamic, kinetic and photochemical considerations, Role of free radicals in atmospheric chemistry.
Chemistry of the stratosphere, Role of UV radiations in production and destruction of ozone, Catalytic decomposition processes with special reference to the role of NO, OH and ClO Radicals, Anthropogenic sources of Cl, formation of Antarctic and Arctic ozone holes.
Smog formation, Chemical species in smog, VOCs and their oxidation, Emissions from two stroke and four-stroke gasoline engines, Emissions from diesel engines, CNG and alternative fuels, Production of ozone in the lower atmosphere and its impact.
Nitrogen and Sulphur species present in the atmosphere and their sources, Production of nitric and sulphuric acids in the atmosphere, Acidifying agents in rain, fog and snow, Control of anthropogenic nitrogen and sulphur emissions - fluidised bed combustion, desulphurisation, SONOX process, Conversion of coal to liquid and gaseous fuels.

Aerosol chemistry, Polyaromatic hydrocarbons (PAHs) and heavy metals in aerosols, Condensation aerosols, the Arctic haze, Lifetime and transport of aerosol particles, Pollutants in the urban atmosphere, Indoor air pollution, Radioactivity and radon pollution.
Energy balance of the earth in terms of black body radiation, Greenhouse gases and their generation from various sources, the global warming potential.

**Unit 3. Hydrosphere Chemistry (20 h)**
Distribution of chemical species in water, The Phosphorous and Sulphur systems, Gases in water, Alkalinity.
Organic matter in water, Humic matter in water - origin, formation and environmental role.
Environmental classification of metals in water, Behaviour of Calcium, Copper and Mercury in the hydrosphere, Formation of complexes between metals and anthropogenic pollutants in water.
Partitioning of small organic molecules between water and soil or sediment. sorption of organic species by soil, octanol-water partition coefficient, Role of clay minerals in the environment.
Wastewater treatment processes, Use of chemical coagulants, Treatment of water containing excessive iron, phosphate, nitrate and fluoride.

**Unit 4. Soil Chemistry (14 h)**
Composition of soil, Chemical weathering, Physical properties of soil - particle size, texture, bulk density, permeability, Chemical properties- Cation Exchange Capacity, $p^H$, macro and micro nutrients, Leachate formation.
Wastes from mining and metal production, Acid Mine Drainage, Sewage sludge, Biogas synthesis, Hazardous wastes and their disposal, Incineration.
Pesticides and their role in the environment, DDT and its fate in the environment.

**Semester III**
**Paper Code: CHM 304**
**Paper Title: Advanced Topics in Chemistry**
**Course Credit: 4**

***Course outcome*:** After learning the course, students will acquire the detailed knowledge on nanochemistry, supramolecular chemistry, advanced topics of pericyclic reactions and will be able to characterize and interpret organic molecules using advanced level of NMR techniques.

**Unit 1. Nanochemistry (20 h)**
Introduction to physics and Chemistry of solids, energy bands: conductor, semiconductor and insulator. Size dependence of properties. Donor, acceptor and deep traps. Exciton.
Methods of measuring properties: crystallography, size of particles, surface structure.
Properties of individual nanoparticles: Metal nanoclusters, semiconducting nanoparticles.
Synthesis of oxide nanoparticles by Chemical method and by thermolysis.
Carbon nanoclusters and nanotubes, application of CNT in fuel cell, catalysis, computer and

as chemical sensors. Polymeric nanofibres, supramolecular structures; nanoparticles organized in/on polymer surfaces.
Magnetic nanostructured particles, electrical and optical properties of nano materials.
Quantum wells, wires and dots. Quantum confinement.

**Unit 2. Supramolecular Chemistry (20 h)**
Introduction to supramolecular chemistry, concepts of host guest chemistry, classification, thermodynamics and kinetic stability, non-covalent interactions, molecular recognition, recognition of anionic substrates, supramolecular reactivity and catalysis, effects of medium, chiral recognition and catalysis.
Molecular receptors for different types of molecules: Crown ethers, cryptands, cyclodextrins, Calixarenes.
Molecular devices: ionic, electronic and switching devices.

**Unit 3. Pericyclic reactions (12 h)**
1, 3 - dipolar cycloadditions–stereochemistry of the reactions. Sigmatropic rearrangement–[m+n] sigmatropic rearrangements of hydrogen and chiral alkyl group. Electrocyclic reactions and cyclo reversions–stereochemistry of the reactions.
Cheletropic reactions–linear and nonlinear cheletropic rearrangement; theories of cheletropic reactions, stereochemistry of the reactions.
The ene reactions–ene reactions of 1,7–dienes, carbonyl enophiles, retro-ene reaction.

**Unit 4. Characterization of organic molecules (12 h)**
Introduction to 2D–NMR. Assignment of $^{1}H$ and $^{13}C$ chemical shifts by using 2D COSY, HSQC and HMBC spectra for simple organic molecules and natural products.
Structure determination of organic compounds using IR, UV-Visible, $^{1}H$ & $^{13}C$ NMR and Mass spectroscopic techniques.

**Semester III**
**Course Code: CHM 305**
**Course Title: Practical (Physical Chemistry)**
**Course Credit: 5**

***Course outcome***: The students will be able to understand physical chemistry from experimental point of view. Moreover, they will learn some modern methods of analysis required in different area of research.

**Unit 1. Chemical Kinetics (20 classes)**

(a) Determine the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using least-squares calculation.
(b) Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
(c) Determine the inversion of sucrose in presence of two acids polarimetrically using Guggenheim plots and hence determine the relative strengths of the acids.

(d) Study the saponification of ethyl acetate by sodium hydroxide and determine the order of the reaction and energy of activation.

(e) Study the autocatalytic reaction between oxalic acid and $KMnO_4$ and determine the order of the reaction.

(f) Study the mutarotation of glucose in presence of acid and base by polarimetric method. Investigate the influence of acid and base strength on the rate of the reaction.

(g) Study the decomposition of kinetic of the formation of complex between sodium sulphide and sodium nitroprusside spectrophotometrically. Determine rate constant and order of reaction.

(h) Study the kinetics of the reaction between peroxydisulphate and potassium iodide and find the influence of ionic strength on the rate constant.

(i) Study the kinetics of the oxidation of ethanol by Cr(VI) and find the rate constant of the reaction. Also find the order of the reaction by half-life period method.

(j) Establish the order of reaction $K_2C_2O_4$ + $2HgCl_2$ to $Hg_2Cl_2$ + 2KCl + $CO_2$ by the method of ratio variation.

**Unit 2. Conductometry (20 classes)**

(a) Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence find the degree of dissociation constant of the acid.

(b) Compare the relative strength of acetic acid and monochloroacetic acid by conductance measurement.

(c) Determine the solubility and the solubility product of a sparingly soluble salt like $PbSO_4$ or $PbI_2$ at room temperature by conductance measurement.

(d) Determine the degree of hydrolysis and the hydrolysis constant of aniline hydrochloride/sodium acetate.

(e) Determine the strength of the components of the following mixtures by conductometric titration.

   (i) Hydrochloric acid and acetic acid.
   (ii) Sulphuric acid and copper sulphate.
   (iii) Hydrochloric acid and potassium chloride.

**Unit 3. $P^H$-metry and Potentiometry (15 classes)**

(a) Determine the dissociation constant of acetic acid/oxalic acid by Albert-Serheart method/using Hendersen's equation.

(b) Find the amount of the components of the following mixtures using PH–metric titration.

   (i) Hydrochloric acid + acetic acid
   (ii) Hydrochloric acid + oxalic acid
   (iii) Potassium chloride + potassium bromide + potassium iodide

(c) Determine the apparent ionisation constant of acetic acid by potentiometric titration of the acid against sodium hydroxide using quinhydrone electrode.

(d) Potentiometrically estimate strengths of solutions of hydrochloric acid and acetic acid individually and a mixture of the two using standard sodium hydroxide solution.

(e) Titrate potentiometrically ferrous ammonium sulphate against potassium dichromate and determine the standard electrode potential of the ferrous/ferric system.

**Unit 4. Spectrophotometry, refractometry and others (15 classes)**

(a) Verify Beer's Law and determine the concentration of solutions like $KMnO_4$/$K_2Cr_2O_7$/$CuSO_4$.

(b) Determine the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
(c) Determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method of continuous variation.
(d) Determine the refractive index of a liquid like carbon tetrachloride and hence find the radius of its molecule.
(e) Verify the mixture law of refraction and draw the calibration curve for mixtures like glycerol/water, *n*-heptane/*n*-hexane. Hence, determine the composition of an unknown mixture of two components.

**Unit 5. Miscellaneous experiments (10 classes)**
(a) Determine the molar mass of a polymer by Viscometric method.
(b) Study the variation of surface tension of a solution of *n*-propyl alcohol/ethanol with concentration and determine the limiting cross-sectional area of the alcohol molecule.
(c) Determine the partial molar volume of methanol/ethanol/formic acid by graphical method by determining the densities of solutions at different concentrations.
(d) Determine the influence of NaCl, naphthalene and succinic acid on the critical solution temperature of phenol-water system using 0.5, 1 and 1.5% concentrations.
(e) Study the complex formation between $Cu^{2+}$ ion and ammonia by distribution method and find the composition of the complex.
(f) Perform theoretical calculations using a computer on
    (i) Least squares fitting and plotting linear and exponential graphs.
    (ii) Charge density distribution and shapes s and p orbitals.
    (iii) Potential energy diagram of hydrogen molecule ion.

***N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.***

**Semester III**
**Paper Code: CHM 306E1**
**Paper Title: Biochemistry**
**Course Credit: 3**

***Course outcome*****:** Students will be able to demonstrate and represent the different chemical and physical processes of living organisms.

**Unit 1. Metabolism (14 h)**
Metabolic processes– catabolism and anabolism; ATP– currency of biological energy; Energy-rich and energy-poor phosphates. Carbohydrate metabolism– Glycolysis, gluconeogenesis, Kreb's cycle.

**Unit 2. Bioorganic Chemistry (16 h)**

(a) Nucleic acids–classification; nucleosides, nucleotides, structures and functions of DNA and RNA, chemical and enzymatic hydrolysis of nucleic acids, DNA-replication and RNA-transcription, introduction to cloning.

(b) Proteins–Aminoacids, primary, secondary, tertiary, and quaternary structure of proteins; biosynthesis of aminoacids, activation of aminoacids, *t*-RNA, ribosomes, *m*-RNA, mechanism of transcription and translation; sequencing of amino-acids in polypeptides.

**Unit 3. Bioinorganic Chemistry (18 h)**

Distribution of metal ions in nature and their biological significance. Iron storage and transport - siderophores, ferritin and tranferrin, $Na^+/K^+$ pump. Dioxygen storage and transport structure and functions of myoglobin, haemoglobin. Electron transfer proteins - structure and function of iron-sulphur proteins, cytochromes and plastocyanine. Metal enzymes - nitrogenases and Dioxygen fixation, vitamin $B_{12}$, Inorganic drugs (gold compounds and cisplatin), chelate therapy.

**Semester III**
**Paper Code: CHM 306E2**
**Paper Title: Computational Quantum Chemistry**
**Course Credit: 3**

***Course outcome***: After learning the course, students will acquire the detailed knowledge on computational quantum chemistry and its applications.

**Unit 1. Many Electron Theory (12 h)**

Indistinguishability of particles; Antisymmetry principle and many electron wave function; Hartree-Fock theory; Roothaan equations, Koopman's theorem; Population analysis; Basis set; Electron correlation.

**Unit 2. (14 h)**

(a**) Radiation-Matter Interaction**: Time-dependent perturbation theory; semi-classical treatment of radiation-matter interaction; Transition probabilities and rates; Einstein's A and B coefficients, selection rules.

(b) **Density Functional Theory**: Hohenberg-Kohn theorem; Kohn-Sham theory; exchangecorrelation functionals.

**Unit 3. Applications (10 h)**
Potential energy surfaces; weak interactions; thermochemistry and kinetics of simple chemical reactions; spectroscopy.

**Unit 4. Introduction to Chemical Reaction Dynamics (12 h)**
Types of chemical reactions; Atom-diatom interaction; Harmonic oscillator model for diatom. The collinear arrangement- Hard sphere model; Reaction cross section and flux density.

**Semester III**
**Paper Code: CHM 306E3**
**Paper Title: Solid State Chemistry**
**Course Credit: 3**

***Course outcome***: After learning the course, students will acquire the detailed knowledge on theories, reactions and properties solid state and materials.

**Unit 1. Solid State Reactions (16 h)**
Preparative Methods: Vapour phase transport, preparation of thin films – electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.
Characterization of Solids: Crystal diffraction of X-rays, X-ray diffraction method; Powder method– principles and uses; Scattering of X-rays by crystals – systematic absences; Electron diffraction; Neutron diffraction.

**Unit 2. Powder Compact Reactions and Solid-State Defects (18 h)**
Diffusion Model: Parabolic rate law, Jander's rate equation, Kroger-Zeigler equation, Ginstling- Brounshtein rate equation.
Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent image formation, lithium iodide battery.
Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Color centers: F-centre, electron and hole centre; colour centre and information storage.

**Unit 3. Magnetic and Optical Properties of Solids (14 h)**
Behaviour of substances in magnetic field; Effects of temperature (Curie & Curie-Weiss laws); Magnetic moments; Mechanism of ferro- and antiferromagnetic ordering– super exchange. Luminescence and phosphors; Configurational coordinate model, Antistoke phosphors, Lasers–ruby and neodymium.

**Semester III**
**Paper Code: CHM 306E4**
**Paper Title: Applied Electrochemistry**
**Course Credit: 3**

***Course outcome***: The students will acquire the detailed knowledge and will be able to demonstrate electrochemical energy conversion and storage processes and surface modification techniques.

**Unit 1. Electrochemical energy conversion and storage (24 h)**

Batteries: History and basics, classification, characteristics with units-voltage, current,capacity, electricity storage density, energy density, power density, energy efficiency, cycle life, shelf life.

Primary batteries: Construction, reactions and uses of Leclanche' dry cell, alkaline Leclanche cell, zinc-silver oxide cell.

Secondary batteries: Construction, working (charge-discharge reactions), applications advantages and of Pb-acid and Ni-Cd batteries.

Hybrid Batteries: Metal-air batteries- meaning, Zn-air battery, Fe-air battery, Charging of metalair battery, Metaloxide-hydrogen/hydride batteries, advantages and limitations of these cells.

Lithium batteries: Primary and secondary lithium battery, Li-ion battery and Lithium ionpolymer battery.

Electrochemical supercapacitors: comparative meaning of capacitor, electrolytic (super) capacitor and ultracapacitors, materials for construction, applications, advantages and limitations.

Fuel cells: Energy efficiency of electrochemical and thermal conversion (Carnot limitation).Definition of fuel cell, classification. Fuel cell efficiency- thermodynamic, electrochemical, practical efficiency. Electrode (anode and cathode) mechanism of fuel cell, Brief description on construction, working principle and applications of each type fuel cells. An account of electrocatalysts, proton exchange membrane (PEM) fuel cells and direct methanol fuel cell.

**Unit 2. Surface Modification techniques (24 h)**

Definition, important processes of metal finishing, technological importance of metal finishing. Electroplating: Definition, theory and mechanism of electroplating, effect of plating variables on the properties of electrodeposits, comparative account of complexing and non complexing baths (general treatment), additives in the plating bath and their significance.

Metallic coating: Preparation of substrate surface, electroplating of Cu and Cr. Applications of Au and Ag platings.

Solar selective coatings: Characteristics, methods of preparation and applications.

Techniques of electroplating: Galvanizing, Anodizing, Phosphating, Chromating.

Electroless plating: Definition, advantages over electroplating, pretreatment of substrates, an account of electroless plating of Ni including applications.

Testing of coats: Principles of measurement of coating thickness, adhesion, porosity, corrosion resistance, reflectance, and hardness.A brief account of surface analysis by XPS and AES techniques.

Indusrtial effluent treatment: An account of removal of toxicants like CN, Cr, Pb and Cd from plating industrial effluent.

**Semester III**
**Paper Code: CHM 306E5**
**Paper Title: Supramolecular Chemistry**
**Course Credit: 3**

***Course outcome***: The students will acquire the detailed knowledge and will be able to demonstrate principles, properties and applications of supramolecular chemistry.

**Unit 1. Supramolecular Chemistry–I (18 h)**
Properties of covalent bonds - bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy, intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. Magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects.Hydrogen bond.
Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextrines.
Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

**Unit 2. Supramolecular Chemistry–II (14 h)**

(a) Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.
(b) Supramolecular reactivity and catalysis.
(c) Transport processes and carrier design.
(d) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

**Unit 3. Dendrimers (16 h)**

(a) Introduction, synthesis and characterization of macromolecular materials, including linear, branched, dedrimetric and star polymers.
(b) Synthetic strategies and stuctural variations. Mechanical and physiochemical properties of polymer types, Kinetics of living polymerization; applications to nanostructures, templates and advanced devices.
(c) Host-guest assembly and supramolecular assembly.
(d) Competitive binding of guest molecules on the surface or in the interior of dendrimers.
(e) Supramolecular structure of dendrimer/surfactant aggregates.

Biomedical applications, biosensing, photodynamic theory, dendrimer-based MRI contrasts.

**Semester IV**
**Course Code: CHM 401**
**Course Title: Polymer Science**
**Course Credit: 4**

***Course outcome***: The students will acquire the detailed knowledge about polymers, their synthesis, processing abilities, properties, structure-property relationship to their applications.

**Unit 1. Polymerization and Kinetics (16 h)**
Step polymerization, chain polymerization including carbonyl polymerization, Ziegler–Natta coordination polymerization, group transfer polymerization, ring opening polymerization, metathesis polymerization, controlled radical polymerization, supramolecular polymerization, Step copolymerization, chain copolymerization, Types of copolymers, Copolymer equation, Monomer reactivity ratios. Structure and reactivity of monomers and radicals, Alfrey price Q-e scheme, Block and graft copolymers.

**Unit 2. Polymer characterization (12 h)**
Chromatographic method, Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis, thermal transition in polymer (Tg, Tm). Physical testing: tensile strength, tear strength, fatigue failure, resilience, hardness, impact and abrasion resistance.

**Unit 3. Structure and Properties (16 h)**
Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting.
Polymer structure and physical properties-crystalline melting point Tm - melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion.
The glass transition temperature Tg: Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking.

**Unit 4. Polymer Processing (10 h)**
Plastics, elastomers and fibres. Compounding reinforcing. Processing techniques: two roll mill mixing, internal mixer, calendaring, die casting, rotational casting, film casting, moulding, extrusion, thermoforming, foaming and fibre spinning.

**Unit 5. Polymer in Special uses (10 h)**
High temperature and fire resistant polymers, Liquid crystal polymers, Conducting polymers, Polyelectrolytes, Biodegradable polymers, Superabsorbent and Self-healing polymer.

**Semester IV**
**Course Code: CHM 402**
**Course Title: Natural Products and Heterocyclic Chemistry**
**Course Credit: 4**

***Course outcome*:** After learning the course, students will be able to identify different types of natural products, their sources and applications. Students will also be able to describe important methods of extraction, their synthesis, and biosynthesis processes.

**Unit 1. Chemistry of carbohydrates (16 h)**
Classification of carbohydrates. Monosaccharides– D- & L- series, acyclic and ring structure of ketoses and aldoses and their configurational representation; anomerization, epimerization and mutarotation; anomeric effect; reactions; methods of ascending and descending the sugar series; conversion of aldose to ketose and *vice-versa*.
Disaccharides– Ring structure of sucrose, maltose, lactose and their hydrolysis.
Polysaccharides– Representative structure of starch, glycogen and cellulose.
Introduction to deoxysugars, glycosides, glycals, glycosamines and glycosans.

**Unit 2. Chemistry of terpenoids (16 h)**
Occurrence and classification; isoprene rule, general methods of structure determination; chemistry including syntheses of the following compounds - caryophyllene, α-santonin, abietic acid, gibberellic acid, longifolene; biogenetic pathway of mono-and sesquiterpenes. Introduction and general reactions; introduction to cholesterol, ergosterol, vitamin $D_1$ and $D_2$; introduction to sex hormones.

**Unit 3. Chemistry of alkaloids (10 h)**
General methods of extraction and structure determination, chemistry including total chiral syntheses of reserpine and morphine.

**Unit 4. Chemistry of porphyrins (10 h)**
Porphyrin ring and chemistry of heme, oxygen transport by haemoglobin, chemistry of chlorophyll and its role in photosynthesis.

**Unit 5. Heterocyclic Chemistry (12 h)**
Nomenclature, π-excessive and π-deficient heterocycles, Principles of heterocyclic synthesis involving cyclization and cycloaddition reaction. Synthesis and properties of three, four, five, six and seven membered heterocycles containing one, two and three heteroatoms *viz.*, N, O and S (aziridine, oxirane, thiirane, azetidine, oxetane, thietane, pyrazole, isoxazole, isothiazole, imidazole, oxazole and thiazole, pyran, azepine, oxepine, thiepine). Elementary idea of Click Chemistry.

**Semester IV**
**Course Code: CHM 403**
**Course Title: Transition Metals and Inorganic Materials**
**Course Credit: 4**

***Course outcome***: Students will be able to explain/describe/rationalize molecular structure and bonding using group theory.

**Unit 1. Application of group theory (16 h)**

Representation of symmetry operators by matrices, representation of groups - reducible and irreducible representations, the Great orthogonality theorem and properties of irreducible representations, Character tables Mulliken notations.

Transformation properties of atomic orbitals, the Direct Product, construction of Hybrid orbitals for $AB_n$ molecules, construction of symmetry adapted linear combinations (SALCs) and MOs of simple $AB_n$ molecules. Selection rules for electronic and vibrational spectroscopy.

**Unit 2. Ligand Field Theory (12 h)**

The d wave functions (orbitals), Crystal field potential, Symmetry aspects of d orbital splitting by ligands. Electron repulsion in many electron atoms, Free ion terms for $d^n$ configurations, Electron repulsion parameters, spin - orbit coupling, Effect of weak crystal field on $O_h$ symmetry on the S, P, D and F terms, Free ions in strong crystal fields. Term energy level diagram for $d^n$ configurations in $O_h$ and $T_d$ symmetries, Tanabe-Sugano diagrams.

Influence of the d-configuration on the geometry and stability of complexes. MO theory of complex compounds, LGO and MOs of $ML_6$ and tetrahedral complexes.

**Unit 3. Electronic spectra (10 h)**

La Porte Selection Rules, Effect of vibronic coupling and spinorbit coupling, band intensities and band widths, Jahn Teller effect. Spectra of aqueous solutions of $M(H_2O)_6^+$, Spectra of high spin and low-spin $ML_6^{n+}$ complexes, Calculation of 10 Dq and values from spectra, distorted octahedral and tetrahedral complexes, M to L and L to M charge transfer spectra.

**Unit 4. Magnetic properties of transition metal ion (10 h)**

Magnetic properties of free ions, spin-only magnetic moments of $d^n$ ions in weak and strong crystal fields of $O_h$ and $T_d$ symmetries, orbital contribution and the effect of spin-orbit coupling, quenching of orbital angular momenta by crystal fields, temperature independent paramagnetism, high-spin low-spin equilibria, Ferromagnetism and antiferromagnetism with examples from metal complexes, Magnetic properties of second and third transition series and the lanthanide elements. Measurement of magnetic susceptibility.

**Unit 5. Inorganic Materials (16 h)**

Magnetic exchange and exchange coupling phenomena, magnetic materials, molecular magnets, ferrofluids. Crystalline, liquid crystalline and amorphous materials, non-stoichiometric oxides, crystal defects, nano materials.

Band theory of metals, semiconductors, *p-* and *n-* type semi-conductor. Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 materials, application of high Tc materials.
Thermoelectric properties - dielectric, ferroelectric, piezo electric materials, solid electrolytes and Fuel Cells.

**Semester IV**
**Course Code: CHM 404**
**Course Title: Catalysis**
**Course Credit: 4**

***Course outcome***: Students will be able to describe the theories and mechanisms of heterogeneous catalysis, and demonstrate the applications of the materials for industrial purposes.

**Unit 1. Theory and Mechanism of Heterogeneous Catalysis (14 h)**
Adsorption and catalysis, mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, volcano principle, shape and size selectivity of catalysts.

**Unit 2. Preparation and Characterization of Industrial Catalysts (16 h)**
Catalyst design methods, catalyst support and preparation of industrial catalyst, supported and unsupported metal catalysts, bimetallic catalysts, characterization of catalysts and their surfaces. Methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity and reactivity.

**Unit 3. Examples of Heterogeneous Catalysts (18 h)**
Clays, zeolites, bimetallic, semiconductor and oxide catalysts, supported catalysts, polymer catalysts. Production and design of industrial catalysts: Materials and methods, precipitated catalysts, impregnated catalysts, skeletal catalysts, fused and molten catalysts, calcination, reduction, shape formation of catalyst particles, optimal shape and size of catalysts particle Promotion and promoters, causes and mechanism of deactivation, poisoning, sintering, prevention of catalyst decay, regeneration of catalysts.

**Unit 4. Catalysis in Petroleum Industry and Environmental Catalysts (16 h)**
Hydrodesulphurization, synthetic gas and production of chemicals from it. Bi-functional catalysts. Non-selective oxidation of hydrocarbon compounds. Manufacture and transformation of hydrocarbons- hydrogenation and isomerization. Catalytic deactivation and reactivation, control of pollution from automobile exhaust, catalytic converters. Abatement of nitrogen oxides and odours, cleaning of industrial effluents.

**Semester IV**
**Course Code: CHM 405**
**Course Title: Organic Synthesis**
**Course Credit: 4**

***Course outcome*:** Students will be able to describe and design organic synthetic strategies.

**Unit 1. Organic Photochemistry (18 h)**
Photochemistry of carbonyl compounds–representation of the excited states of ketones, photolysis of saturated and *β,γ*- unsaturated ketones. Photoreduction of saturated, arylalkyl and *α,β*-unsaturated ketones and *p*-benzoquinone; Paterno-Buchi reaction, [2+2]-cycloaddition, reactions of singlet oxygen- photooxidation, ene reaction, synthetic applications of singlet oxygen.
Olefinic photochemistry–photostereomutation of cis-trans isomers, optical pumping, [2+2] cycloaddition. Photochemistry of conjugated polyenes - cycloaddition and dimerization of 1,3-butadiene, photochemistry of vision.
Photorearrangements–di-π-methane rearrangement, Photo-Fries rearrangement and photorearrangement of cyclohexadienones, Barton rearrangement.

**Unit 2. Formation of carbon-carbon single bonds (14 h)**
Alkylation–importance of enolate anions, alkylation of activated methylene groups, dianion in synthesis, alkylation of ketones, enamine and related reactions; alkylation of thio-and seleno-carbanions; allylic alkylation of alkenes, Michael addition (conjugate addition).
Aldol reaction–use of boron and silyl enolates; directed aldol reaction.
Synthetic applications of carbene and carbenoids; formation of carbon-carbon bond by addition of free radicals-to alkenes; photocyclization reactions.

**Unit 3. Formation of carbon-carbon double bond (16 h)**
Elimination reactions–acid catalysed dehydration of alcohols, solvolytic and base-induced elimination from alkyl halides & sulphones, Hofmann elimination from quaternary ammonium salts.
Pyrolytic syn elimination–pyrolyses of carboxylic esters and xanthates (Chugaev reaction) and amine oxides (Cope reaction).
Wittig and related reactions–use of stabilized and unstabilized phosphorus ylides, Peterson reaction.
Alkenes from sulphones, decarboxylation of lactones, stereoselective synthesis of tri and tetrasubstituted alkenes.

**Unit 4. (16 h)**
(a) *Synthetic application* of *Organometallics and activation* of *C-H bonds*
Preparation, stability, reactivity and synthetic applications of organo-lithium, tin, copper, zinc and palladium reagents.
Hofmann-Loeffler-Freytag reactions, cyclisation reactions of nitrenes, Barton reaction and related processes, photolysis of hypohalides, reactions of monohydric alcohols with lead tetraacetate.

(b) *Designing Organic Synthesis*
Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and

convergent synthesis, umpolung of reactivity and protecting groups.

**Semester IV**
**Course Code: CHM 406**
**Course Title: Organometallics and Photoinorganic Chemistry**
**Course Credit: 4**

***Course outcome***: Students will be able to discuss/explain the synthesis, structure, & reactivity of organometallic compounds, reagents, and demonstrate their uses in industrially important reactions.

**Unit 1. Nature of metal-carbon bonds in transition metal compounds (10 h)**
Classification of organometallic compounds, M–C $\sigma$ bond in metal alkyls, $\beta$-hydrogen elimination. Complexes with metal carbon $\pi$-bonds - with olefins, acetylenes, allylic groups and dienes– electronic structure and bonding. Bonding in metal carbocyclic systems cyclopentadienyl and other carbocyclic ligands, MO treatment of bonding in ferrocene based on symmetry properties of the ligand and metal orbitals. Bonding in carbene and carbine complexes.

**Unit 2. Synthesis, structure and properties of organometallic complexes (16 h)**
Olefin complexes, acetylene complexes, complexes formed by polyenes and allylic compounds -synthesis and relevance. Cyclopentadiene and arene metal complexes– general reactions. Transition metal alkyls and ylides complexes, metal carbene and metal carbyne complexes -synthesis and reactivity.
Synthesis of metal carbonyls and metal carbonyl hydrides reactions and synthetic utilities. High nuclearity carbonyl cluster, structures, electron counting schemes and bonding - Wade's rules (isolobal analogy).

**Unit 3. Fundamental reactions of organotransition metal complexes (12 h)**
Ligand co-ordination and dissociation - displacement reaction in square planar complexes, steric and electronic influences of ligands. Oxidative addition and reductive elimination. Insertion reactions- insertion of CO, alkenes. Reaction of co-ordinated ligands- reactions of co-ordinated olefins, acetylenes and arenes.

**Unit 4. Organometallics in catalysis (16 h)**
Homogeneous and heterogeneous catalysis. Polymerization and oligomerization of olefins and dienes. Hydrogenation, hydroformylation, isomerization, metathesis and carboxylation of olefins. Synthesis of acetic acid from methanol, reactions of synthesis gas. Oxidation of olefins by Wacker process, synthesis of acrylates, olefin epoxidation. C-H bond activationhydroxylation and autoxidation - basic idea. Allylic oxidations.

**Unit 5. Photoinorganic chemistry (10 h)**
Ligand field and charge transfer states (Thexi and DOSENCO states), Energy dissipation by radiative and non-radiative processes, Jablonski diagram. Photosubstitution on Cr(III) and Co(II) compounds, cis-trans isomerisation, metal carbonyls. Photoredox reactions of Co(III) complexes, Photo catalysis and solar energy conservation by $Ru(bpy)_3^{2+}$.

**Semester IV**
**Course Code: CHM 407**
**Course Title: Chemistry of Surfactants**
**Course Credit: 4**

***Course outcome***: The students will be able to demonstrate the chemistry of surfactants including their importance and applications.

**Unit 1. Introduction (18 h)**
Characteristic Features of Surfactants: General structural features & behavior of surfactants, classification of surfactants, hydrophobic/solvophobic interaction, Kraft point.
Adsorption of Surfactants: Adsorption at solid/liquid, liquid/gas and liquid/liquid interfaces, Gibbs adsorption equation, adsorption isotherms, effect of added electrolyte on the surface excess of ionic surfactants.

**Unit 2. Micelles (16 h)**
Micelle formation by surfactants: Critical micelle concentration, cmc meaurement, conductance behaviour of ionic micellar solution, micellar structure and shape, factors affecting cmc, temperature dependence of cmc, thermodynamics of micellization, counterion binding constant.

**Unit 3. Mixed Surfactants (14 h)**
Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, Rubingh's treatment, Rodenas treatment, conterion binding in mixed surfactants.

**Unit 4. Solubilisation and Emulsification (16 h)**
Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions, reactions in micellar and microemulsion media.

**Semester IV**
**Course Code: CHM 408**
**Course Title: Bioorganic and Medicinal Chemistry**
**Course Credit: 4**

***Course outcome*:** Students will be able to identify, compare and explain aspects related to biochemical processes, drug design and mode of action of drug.

**Bioorganic Chemistry**
**Unit 1.1. Biochemistry of Lipids (10 h)**
Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies. Biosynthesis of fatty acids, triacylglycerols, phospholipids, cholesterol and related steroids; prostaglandins.

**Unit 1.2. Chemistry of vitamins (10 h)**
Carotenoids - classification, chemistry of $\beta$-carotene, lycopene and canthaxanthin. Synthesis of $\beta$-carotene, provitamin A, singlet oxygen quenching and food coloring properties of carotenes. Classification and functional role in biological systems; chemistry of thiamine, riboflavin, retinol, tocopherols, vitamin C and pyridoxine.

**Medicinal Chemistry**
**Unit 2.1. Introduction to Basic Concepts (10 h)**
Definition of drugs and factors affecting their bioactivity; definition chemotherapeutic index and therapeutic index; theoretical aspects of drug-receptor interaction, the two-state Model of Receptor Theory; QSAR, drug agonist and antagonist; pharmaco-kinetics and pharmacodynamics; mechanism of drug action.
Lead compound, molecular modification; elementary idea of molecular modelling of drug; introduction to combinatorial library of drugs.

**Unit 2.2. Sulphadrugs (10 h)**
Historical significance of sulpha drugs as antibacterial agents; introduction to sulphanilamide and other important sulpha drugs and their mode of action.

**Unit 2.3. Antibiotics (14 h)**
Introduction and classification. $\beta$-Lactam antibiotics –Natural and semisynthetic penicillins, their structure-action relationship and chemical modification, penicillins sensitive and resistant to penicillinase; mode of action of $\beta$-Iactam antibiotics.
Aminoglycoside antibiotics–Streptomycin, gentamycin, kanamycin, neomycin and their mode of action.
Tetracyclines–Structure-action relationship and therapeutic uses.
Chloramphenicol–Synthesis and characterization, mode of action. Introduction to macrolide and peptide antibiotics.

**Unit 2.4. Antimalarials (10 h)**
Classification of humane malaria and plasmodia responsible for them, life cycle of plasmodia; quinine, chloroquine, trimethoprim, mefloquin-their structure and activity as antimalarial; artemisinin and its derivatives, structure-action relationship.

**Semester IV**
**Course Code: CHM 409**
**Course Title: Bioinorganic Chemistry**
**Course Credit: 4**

***Course outcome***: Students will be able to classify/critically examine supramolecular systems, explicate the underlying principles, with regard to concepts of molecular recognition, self-assembly, catalysis, and devices. They will also learn the role of metal ions in functioning of biological systems, toxicity due to metal ions, the role in a diseases and therapy.

**Unit 1. Supramolecular Chemistry and Ion Transport (16 h)**
Definition and examples of Supramolecules, Self-assembly and membranes, Molecular receptors- Cryptands, Valinomycine, Spherands, Molecular recognition. Interaction of metal

ions and metal complexes with DNA.
Supramolecular Transport: Active transport of ions across cell membranes, Selectivity of Na and K with crown ethers, cryptands and ionophores, Na/K pump; Transport of $Ca^{2+}$, Bio-minerals containing Ca and Fe; Transport and Storage of Iron; Transferrins, Sideraphores, and Ferritin.

**Unit 2. Carrier, Transport, Storage and Activation of Dioxygen (16 h)**
Active site structure and function of oxygen carrying proteins: Metalothionins and Ceruloplasmin. Haemoglobin, Myoglobin, Haemerythrin and Haemocyanine; $O_2$ binding equilibria and mechanism of cooperativity in Hemoglobin, Design of Model $O_2$ carriers, Reaction leading to toxicity due to dioxygen. Oxidases and Oxygenase: Catalase, Peroxidase, Superoxide Dismutase, Cytochrome *c* Oxidase, Cytochrome P-450, and Pyrocatechol Dioxygenase - their biological functions, role of metal and dioxygen reactivity.

**Unit 3. Metalloenzymes (12 h)**
Structure and function of carboxypeptidase A and carbonic anhydrase. Importance of Co(II) substitution in Zn proteins; Structure and function of co-enzyme $B_{12}$. Role of Ni, Cr and V in enzymes; Molybdenum enzymes, structure and function of Nitrogenase, chemistry of dinitrogen fixation, Xanthine oxidases.

**Unit 4. Electron transfer proteins (10 h)**
Metalloproteins in the electron transfer chains in membrane, The Cytochromes (*a, b, c* types), Mechanism of electron transfer reactions in proteins; Iron Sulfur proteins–Rubredoxin, Ferredoxin, and HiPIP.

**Unit 5. Metals in medicine (10 h)**
Metal deficiency and disease, toxic effect of metals - Fe and Cu overload, Thalassemia, toxicity due to Hg, As, Cd, and Pd; Chelation therapy (EDTA, BAL, Penicillamine); Gold compounds in Rh. arthritis, Cisplatin and related Anticancer drugs.

## Semester IV
## CHM 410: Project/Dissertation
## Course Credit: 6

***Course outcome***: The students would be able to demonstrate and plan a scientific research, and implement it within a reasonable time-frame. It is expected that after completing this project/dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental works. In addition, students will be able to handle laboratory equipment and chemicals, and utilize sophisticated instruments for analysis, data collection and interpretation. Moreover, students will learn how to perform literature review and will be able to critically examine research articles, and improve their scientific writing/communication.

**RECOMMENDED BOOKS & REFERENCES**

**A. *PHYSICAL CHEMISTRY***


1. Atkins, Peter W.; de Paula, Julio (2010). Physical Chemistry (9th ed.). Oxford University Press.
2. Levine, I. (2008). Physical Chemistry (6th ed.), McGraw–Hill Science.
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4. Textbook of Physical Chemistry, A.W. Adams
5. Quantum Chemistry, I.N. Levine
6. Pilar F.I. (2001) Elementary Quantum Chemistry (2nd Ed.), Dover Publication, Inc.
7. Chandra, A.K. (1994) Introductory Quantum Chemistry (16th Reprint.). TataMcGraw-Hill,
8. Coulson's Valence, R. McWeeny.
9. Valency Theory, Murrel, Kettle and Teddler
10. Atkins, Peter W.; Friedman, Ronald (2005). Molecular Quantum Mechanics (4th ed.), Oxford University Press.
11. Quantum Chemistry, Mcquarrie
12. Heat and Thermodynamics, Zemansky
13. Statistical Thermodynamics, M.C. Gupta (New Age International)
14. Modern Electrochemistry, Bokris and Reddy, Vols. 1&2 (Butterworth)
15. Chemical Kinetics, K.J. Laidler
16. Reaction Kinetics, Pilling and Seakins (OUP)
17. Textbook of Polymer Science, F.W. Billmeyer
18. Polymer Science, Gowarikar, Viswanathan and Sreedhar
19. Principles of the Solid States, H.V. Keer
20. Physical Chemistry through Problems, Dogra and Dogra
21. Thermodynamics, Randall, Pitzer and Brewer
22. Chemical Thermodynamics, E.N. Yeremin
23. Non-Equilibrium Thermodynamics, D.D. Fitts
24. Homogeneous Catalysis, Parshall and Ittel (Wiley)
25. Heterogeneous Catalysis, Principles & Applications, G.C. Bond
26. Introduction to the principles of Heterogeneous Catalysis, Thomas and Thomas
27. Catalysis by Metals, G.C. Bond.
28. New methods of catalyst preparation and characterization, G.C. Bond and P.A. Germer
29. Catalysis, J.C. Kurlakose
30. Heterogeneous Catalysis, D.K.Chakrabarty
31. Catalysis: Science and Technology, J.R. Anderson and M. Boundart
32. Principles of Biochemistry, A. Lehninger
33. Outlines of Biochemistry, Cohn and Stumpf
34. Rates and Mechanism of Chemical Reactions, Gardiner W.G (W.A. Benjamin Inc.)
35. Kinetics and Mechanism, Frost A.A and Pearson R.G (Wiley Eastern)
36. Kinetics and Mechanism of Chemical Transformations, Kuriacose R (McMillan, India)
37. Fundamentals of Photochemistry, Rohatgi-Mukherji (Wiley Eastern)
38. Photochemistry, Lalverts and Pitts
39. Principles of Electrochemistry, Koryto J and Dvorak
40. Principles of Polymer Chemistry, Flory P.J
41. Textbook of Polymer Science, Billimeyer F.W
42. Physical Chemistry of Macromolecules, Tanford C
43. Inorganic Polymers, Stone and Graham

44. Introduction to Polymers, Young R.J
45. Physical Chemistry of Polymers, Tagger A.

**B. *ORGANIC CHEMISTRY***

1. Organic Synthesis by Michael B. Smith, McGraw-Hill International Edition
2. Advanced Organic Chemistry by Jerry March, Wiley Eastern Edition
3. Organic Reactions and their Mechanisms by P.S. Kalsi, New Age International
4. Reaction Mechanism by Peter Syke
5. Chemical Hardness by R.G. Pearson, Wiley-VCH
6. Stereochemistry of Organic Compounds by Eliel and Wilen, Wiley & Sons
7. Stereochemistry of Organic Compounds: Principles and Applications by Nasipuri, Wiley & sons
8. Organic Chemistry by Pine, McGraw-Hill International Edition
9. Lehninger Principles of Biochemistry by David L. Nelson and Michael M. Cox, Macmillan Worth Publishers
10. Biological Chemistry by Mahler and Cordes, Harper International
11. Fundamentals of Biochemistry by A.C.Dev, New Central Book Agency (P) Ltd
12. Enzymatic Reaction Mechanisms by C. Walsh, Freeman & Company
13. Some Modern Methods of Organic Synthesis by Carruthers, Cambridge University Press
14. Molecular Orbitals by Lehr and Merchand
15. Importance of Antibonding Molecular Orbitals by Jaffe and Orchin
16. Organic Spectroscopy by William Kemp by ELBS
17. Spectroscopic methods in Organic Chemistry by Williams and Fleming, McGraw-Hill Book.
18. Spectroscopic Identification of Organic Compounds by Silverstein, Bassler and Morril, Wiley & sons.
19. Mass Spectrometry by Reg Davis and Martin Freason, Wiley & sons
20. Organic Chemistry by I.L.Finar, Longman Group Ltd
21. Introduction to Medicinal Chemistry by Alex Gringauz, Wiley-VCH
22. Medicinal Chemistry- An Introduction by Gareth Thomas, Wiley & sons
23. Organometallic Chemistry by Mehrotra and Singh, Wiley Eastern Ltd.
24. Principles of Organometallic Chemistry by P. Powel, Chapman & Hall
25. Designing Organic Synthesis: A Programmed Introduction to Synthon Approach by Stuard Warren, Wiley & sons.
26. The Logic of Chemical Synthesis by Corey and Cheng, Wiley & sons
27. Classics in Total Synthesis: Targets, Strategies and Methods by Nicolaou and Sorensen
28. New Horizons in Organic Synthesis by Nair and Kumar, New Age International
29. Organic Chemistry by Gilman (four volumes)
30. Natural Products by Nakanishi
31. Terpenoids-series of three volumes by Simonsen, Mayo and Pindar
32. Alkaloids- two volumes by Dalton and Boutley
33. Heterocyclic Chemistry: Synthesis, Reactions and Mechanisms by R. K. Bansal, Wiley Eastern Ltd.
34. Organic Chemistry by P.Y. Bruice, Prentice-Hall International
35. Organic Chemistry by R.V. Hoffman, Oxford University Press
36. Organic Chemistry by Sundberg
37. Organic Chemistry by Norman
38. Natural Products: Chemistry and Biological Significance, J. Mann, Fl.S.Davidson, J.B.Hobbs, D.V. Banthrope and J. B. Harborne, Longman,Essex.

39. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
40. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed.Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
41. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.l. Choudhary, Harwood Academic Publishers.
42. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
43. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
44. An Introduction to Drug Design, S. S. Pandeya and J. Fl. Dimmock, New Age International.
45. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14). Ed. M. E. Wolff, John Wiley.
46. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.

**C. *INORGANIC CHEMISTRY***

1. Advanced Inorganic Chemistry by Cotton, Wilkinson Murillo and Bochman
2. Atkins, Peter W.; Shriver, D. F. (2010). Inorganic Chemistry (5th ed.). W. H. Freeman.
3. Inorganic Chemistry: Principles of Structure and Reactivity by Hucheey, Keiter & Keiter
4. Theoretical Inorganic Chemistry by M.C.Day and J.Selbin
5. Chemical Application of Group Theory by F.A.Cotton
6. Structural Inorganic Chemistry by A.F.Wells, Oxford Science Publishers
7. Chemistry of the Elements by Greenwood and Earnshaw
8. Modern Inorganic Chemistry by W.L.Jolly, McGraw-Hill
9. A New Concise Inorganic Chemistry by J.D.Lee, Van Nostrand
10. Introduction to Ligand Fields by B.N. Figgis
11. Multiple Bonds between Metal Atoms by F.A.Cotton and R.A.Walton
12. Comprehensive Coordination Chemistry, Vol-I
13. Magnetochemistry by R.L.Carlin
14. Physical Inorganic Chemistry by S.F.A.Kettle
15. New Direction in Solid State Chemistry by C.N.R.Rao and J. Gopalakrishnan, Cambridge University Press.
16. Solid State Chemistry and its Applications by A.R.West, Wiley & sons
17. Chemistry of Advanced Materials: An Overview by L.V.Interrante and M.I.Hamden-Smith.
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19. Solids and Surfaces: A Chemist's View of Bonding in Extended Structures by R.Hoffman
20. Inorganic Materials by D.W.Bruce and D.O.Hare, Wiley & sons
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**D. *BIOCHEMISTRY***

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2. Biochemistry by L.Freeman, W.H.Freeman
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4. Biochemistry: The Chemical Reactions of Living Cells by D.E.Metzler, Academic Press
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**E. *SUPRAMOLECULAR CHEMISTRY***

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3. Supramolecular Chemistry: Concepts and Perspectives- Jean M. Lehn, VCH
4. Supramolecular Chemistry– Paul D. Beer, Philip A. Gale and David K. Smith; (Oxford Chemistry Primer).

**F. *NANOCHEMISTRY***

1. Nanomaterilas and Nanochemistry, Bréchignac C., Houdy., and Lahmani M. (Eds.) Springer Berlin Heidelberg New York, 2007.
2. Nanoparticle Technology Handbook, Hosokawa M., Nogi K., Naito M and Yokoyama T., (Eds.) First Edition 2007, Elsevier.
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**G. *GREEN CHEMISTRY***
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**H. *ENVIRONMENTAL CHEMISTRY***
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**I. *ANALYTICAL CHEMISTRY***
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