

DEPARTMENT OF CHEMISTRY
SARBATI DEVI WOMEN'S COLLEGE, RAJGANGPUR
PO, CO, PSO- NEP-2020

CORE-I PAPER-I: Atomic Structure, Periodicity of elements and
Chemical Bonding

Course Objectives:

To provide the fundamental knowledge on the structure of atom, which is a necessary pre-requisite in understanding the nature of chemical bonding in compounds. Various types of periodic properties and bondings have been reviewed to strengthen students for grasping this tricky topic and effectively tackle exam questions. The basics of acid-base titrimetric analysis has been incorporated in order to develop the analytical skills of the students.

Course Outcomes:

1. Solve the conceptual questions using the knowledge gained by studying the quantum mechanical model of the atom.
2. Learn the various atomic properties of atoms and their variations in the periodic table.
3. Gain the idea of different types of bonding and their associated properties.
4. Understand the theory and applications of various acid-base titrations.

SYLLABUS

(C L P = 3 3 0; Total Hours = 15 x 3 = 45)

UNIT – I (12 Hours)

Atomic structure:

Rutherford's nuclear model of atom, Bohr's theory and the origin of hydrogen spectrum, Sommerfeld's extension of Bohr's theory, de-Broglie equation, Heisenberg's Uncertainty Principle and its significance. Postulates of wave mechanics, Derivation of Schrödinger's wave equation for hydrogen atom, significance of ψ and ψ^2 . Radial and angular wave functions, Radial function plots, radial probability distribution plots, angular distribution curves. Shapes of s-, p-, d- and f-orbitals, Relative energies of orbitals. Slater's rule and its limitations, Quantum numbers and their significance. Pauli's Exclusion Principle, Hund's rule of maximum spin multiplicity and Aufbau principle.

UNIT – II (10 Hours)

Periodicity of elements:

Introduction to long form periodic table, Cause of periodicity, Division of elements into s-, p-, d- and f-blocks. Atomic radius, ionic radius, covalent radius and Van der Waals radius. Periodic trends in ionic and covalent radii. Ionization energy, electron affinity, electronegativity, and their variations in the periodic table. Applications of electronegativities. Pauling's/Mulliken's scale of electronegativity, Sanderson's electron density ratio.

UNIT – III (10 Hours)

Chemical bonding-I:

Ionic bond-General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Lattice energy, Born-Haber cycle and its application, Born-Landé equation, Madelung constant, importance of Kapustinskii equation for lattice energy. Solvation energy, Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

UNIT – IV (13 Hours)

Chemical bonding-II:

Covalent bond-Valence shell electron pair repulsion (VSEPR) theory, shapes of the following simple molecules and ions containing lone pairs and bond pairs of electrons: CH₄, H₂O, NH₃, PCl₃, PCl₅, SF₆, ClF₃, I₃⁻, BrF₂⁺, PCl₆⁻, ICl₂⁻, ICl₄⁻, NH₄⁺, PO₄³⁻ and SO₄²⁻. Valence Bond theory (Heitler-London approach). Hybridization, equivalent and non-equivalent hybrid orbitals. Ionic character in covalent compounds: Dipole moment. Percentage ionic character from dipole moment and electronegativity difference, Molecular orbital diagrams of homo- & hetero-diatomic molecules (N₂, O₂, C₂, B₂, F₂, CO, NO) and their ions. Calculation of bond order. Concept of bent rule.

Calibration and use of apparatus

Preparation of solutions of different Molarity/Normality.

Estimation of oxalic acid using standard NaOH solution

Estimation of sodium carbonate using standard HCl.

Estimation of carbonate and hydroxide present together in a mixture.

Estimation of carbonate and bicarbonate present together in a mixture.

Metallic bond:

Concept of metallic bond, The free electron model, The valence bond model, The band model (molecular orbital approach), semiconductor and insulators.

Hydrogen bond:

Concept of hydrogen bond, nature of hydrogen bonding, consequences of hydrogen bonding and its importance.

Lab Work

Credit-01

(C L P = 1 0 1; Total Hours = 15 x 2 = 30)

(Laboratory periods: 30 Hours, 15 classes of 2 hours each)

List of experiments

1. Calibration and use of apparatus
2. Preparation of solutions of different Molarity/Normality.
3. Estimation of oxalic acid using standard NaOH solution
4. Estimation of sodium carbonate using standard HCl.
5. Estimation of carbonate and hydroxide present together in a mixture.
6. Estimation of carbonate and bicarbonate present together in a mixture.

Core- I (Paper-II)

Fundamental Organic Chemistry

Course Objectives:

To provide the fundamental knowledge on organic chemistry in order to comprehend other organic chemistry courses in coming semesters with greater depth. The purpose of this core paper is to review the basic concepts of electron displacement and the chemistry of aliphatic and aromatic hydrocarbons. Stereochemistry is also introduced to help to student to visualize the organic molecules and their spatial arrangement in three dimensional spaces and hands on experience on detection of organic molecules.

Course Outcomes:

1. Understanding the basic concepts of electronic displacement phenomena in organic molecules, various bond breaking processes and types of organic reactions.
2. Fundamental knowledge on symmetry and asymmetry aspect of organic molecules and their spatial arrangements in two-dimension and three-dimension with their stereochemistry.
3. Learning the synthesis, structure and stability of unsaturated hydrocarbons, understanding the concept of aromaticity and chemical reactions of unsaturated hydrocarbons and aromatic hydrocarbons.
4. Knowledge on selection of suitable solvent for purification and separation of organic compounds and detection of various elements present in it.

Syllabus

Lecture-Credit-03 (45 Hrs)

Unit-I:

Basics of Organic Chemistry (11 hrs)

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications in dipole moment; organic acids and bases; their relative strength. Homolytic and heterolytic fission with suitable examples. Curly arrow rules; Electrophiles and Nucleophiles; Nucleophilicity and basicity; Types, shape and relative stability of carbocations, carbanions, free radicals and carbenes.

Introduction to types of organic reactions with suitable examples: Addition, Elimination, Substitution, Rearrangement and Pericyclic reactions.

Carbon-carbon sigma bonds, chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Corey-House Reactions, Free radical substitutions: Halogenation –relative reactivity and selectivity.

Unit–II:

Stereochemistry (13 hrs)

Concept of Chirality/Asymmetry, Geometrical isomerism and Optical Isomerism: Optical Activity, Specific Rotation. Determination of Relative and absolute configuration in chiral molecules using D/L, R/S, cis/trans, Syn/Anti and E/Z descriptors using C.I.P rules.

Representation by Fischer Projection, Newmann and Sawhorse Projection formulae in molecules containing one and two chiral-centres. Enantiomers, Distereoisomers, meso-structures, Racemic mixture and their resolution.

Stability and Conformational analysis: types of cycloalkanes and their relative stability, Baeyer strain theory, Conformational analysis of alkanes (ethane and n-butane): Relative stability with energy diagrams. Energy diagrams of cyclohexane: Chair, Half chair, boat and twist boat forms.

Unit–III:

Chemistry of Unsaturated Hydrocarbons (13 hrs)

Carbon-Carbon Pi Bonds: Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/AntiMarkownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, syn and anti-hydroxylation (oxidation). 1,2- and 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

Unit–IV:

Chemistry of Aromatic Hydrocarbons (8 hrs)

Aromaticity: Hückel's rule, aromaticity in benzenoid and non-benzenoid compounds, cyclic carbocations/ carbanions and heterocyclic compounds with suitable examples.

Electrophilic aromatic substitution with mechanism: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the functional groups.

LAB WORK- Credit-01 (15 classes of 2 hours each)

List of Experiments

Detection of extra elements (N, Cl, Br, I and S) in organic compounds by Lassaigne's test.

Functional group tests for alcohols, phenols, carbonyl and carboxylic acid groups in known organic compounds.

Separation and purification of any one component of following binary solid mixture (Benzoic acid/*p*-Toluidine; *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotoluene/*p*- Anisidine) based on the solubility in common laboratory reagents/solvents like water (cold, hot), ethanol (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO₃ etc.

Determination of melting point and boiling point of different organic compounds

CORE-I PAPER-III

States of matter, and Ionic equilibrium

Course Objectives:

The objective of this course is to develop basic and advance concepts regarding gases and liquids. It aims to study the similarity and differences between the two states of matter and

reasons responsible for these. The objective of the practical is to develop skills for working in physical chemistry laboratory. The student will perform experiments based on the concepts learnt in Physical chemistry-I course.

Course outcomes:

- Derive mathematical expressions for different properties of gas and liquid and understand their physical significance.
- Apply the concepts of gas equations and liquids while studying other chemistry courses and understand the importance of pH in every-day life.
- Understand different lattice systems and apply working principles of XRD for understanding crystal structure by powder and single crystal method.
- Handle stalagmometer and Ostwald viscometer properly and determine the density of aqueous solutions. Data reduction, interpretation using numerical and graphical methods.

SYLLABUS

Lecture-Credit 03 (45 hours)

Unit-I: Gaseous state (13 hour)

Kinetic molecular model of a gas, Collision frequency, Collision diameter, Collision cross section, Mean free path and viscosity of gases, including their temperature and pressure dependence, Relation between mean free path and coefficient of viscosity, Maxwell distribution of molecular velocities (no derivation); average, root mean square and most probable velocities and average kinetic energy, Law of equipartition of energy, Behaviour of real gases: Deviations from ideal gas behaviour, Causes of deviation from ideal behavior, Vander Wall equation and its application, Compressibility factor Z, and its variation with pressure for different gases, Critical Phenomenon and critical constant derivation.

Unit-II: Liquid state (10 hour)

Qualitative treatment of the structure of the liquid state; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Capillary action in relation to cohesive and adhesive forces, Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

Unit- III: Solid state (12 hour)

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analyses of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals (stoichiometric and non- stoichiometric).

Unit-IV: Ionic equilibria (10 hour)

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono- and diprotic acids. calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts and its application.

LAB WORK
Credit 01 (15 classes of 2 hours each)

List of experiments:

1. Determine the surface tension by (i) drop number (ii) drop weight method.
2. Study the variation of surface tension of detergent solutions with concentration and determination of CMC
3. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
4. Study the variation of viscosity of sucrose solution with the concentration of solute.
5. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
6. Preparation of buffer solutions of different pH (i) Sodium acetate-acetic acid (ii)
7. Ammonium chloride-ammonium hydroxide
8. Determination of dissociation constant of a weak acid.
9. Determination of solubility product of PbI_2 by titrimetric method.

CORE-I PAPER-IV

Chemical thermodynamics, equilibrium, and Colligative property

Course Objectives:

The learners should be able to apply principles and laws of thermodynamics to reversible and irreversible systems. In addition, they should be able to use spectroscopic data to calculate thermodynamic properties of ideal & real mixtures. In addition, understand the change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Also able to identify factors affecting equilibrium constant using the principles and techniques of statistical thermodynamics.

Course outcomes:

By the end of the course, the students will be able to:

- Discuss the laws of thermodynamics and applications to natural phenomena.
- Acquire a strong foundation of partial molar properties, its variation with temp and pressure for different systems and able to apply on the thermodynamics of simple mixtures.
- Inculcate firm foundations in the fundamentals and application of chemical equilibrium, and ΔG derive the relationship between different equilibrium constants.
- Understand the basic concept of Solutions of non-volatile solutes, colligative properties. Calculate various thermodynamic properties ($\Delta H_{\text{neutralization}}$, $\Delta H_{\text{hydration}}$ & C_v) for chemical reactions using calorimeter.

- **SYLLABUS**
- **Lecture-Credit 03 (45 hours)**

- **Unit-I: Chemical thermodynamics (10 hours)**

- Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics. First law: Concept of heat, q , work, w , internal energy, U , and statement of **first law**; enthalpy, H , relation between heat capacities, calculations of q , w , U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

- **Unit-II (12 hours)**

- Carnot cycle, efficiency of heat engine, Carnot theorem; **Second Law**: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes. **Third Law**: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules. Free Energy Functions: Gibbs and Helmholtz energy; variation of S , G , A with T , V , P ; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters, inversion temperature, Gibbs-Helmholtz equation, Maxwell relations, thermodynamic equation of state.

- **Unit-III : Systems of variable composition (13 hours)**

- Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. **Chemical equilibrium**: Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient (van Hoff's reaction). Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p , K_c and K_x . Le Chatelier principle (quantitative treatment) and its applications.

- **Unit-IV Solutions and Colligative Properties (10 hours)**

- Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties: (i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

LAB WORK- credit 01 (15 classes of 2 hours each)

List of experiments

1. Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
2. Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Calculation of the enthalpy of ionization of ethanoic acid.
4. Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

5. Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
6. Determination of enthalpy of hydration of copper sulphate.
7. Determination of heat of solution (ΔH) of oxalic acid/benzoic acid from solubility measurement.

CORE-I PAPER-V

Acids and Bases, Metallurgy, Chemistry of main group elements

Course Objectives:

To provide the basic knowledge on general principles of acids and bases, principle of metallurgy and chemistry of s- and p-block elements. Students can learn about chronological developments of the concepts of acids and bases. It will help students to get aware of the pH scale and classify a substance as acidic, basic, or neutral based on their pH or hydrogen ion concentration. Students can achieve the knowledge regarding volumetric analysis and preparation of metal complex.

Course Outcomes:

1. Know how the various theories of acid and base, and understand the occurrence and purification of metals
2. Learn the different properties of s- and p-block elements
3. Understand the preparation and properties of inorganic polymers.
4. Achieve knowledge on how to standardize, estimate and prepare inorganic compounds/metal ions.

SYLLABUS

(C L P = 3 3 0; Total Hours = 15 x 3 = 45)

UNIT – I (10 Hours)

Acids and Bases

Different concepts of acids and bases: Arrhenius theory, Bronsted-Lowry theory, Lewis theory, The Lux-Flood definition, The Usanovich definition, acids and bases in proton solvents, Concept of conjugate acid and conjugate base, Concept of pH, Pearson's classification of Lewis acid and Lewis bases into Hard and Soft Acids and Bases (HSAB), HSAB principle, application of HSAB principle.

Principle of metallurgy

Chief modes of occurrence of metals, Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent, electrolytic reduction, hydrometallurgy. Methods of purification of metals: electrolytic process, parting process, Van Arkel-de Boer process, Mond's process and Zone refining.

UNIT – II (12 Hours)

Chemistry of s-Block Elements

General characteristics: melting point, flame colour, reducing nature, diagonal relationships and anomalous behavior of first member of each group. Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water. Common features such as ease of formation, thermal stability and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, and sulphates. Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; Hydride and their classifications: ionic, covalent and interstitial, EDTA complexes of calcium and magnesium. Solutions of alkali metals in liquid ammonia and their properties.

UNIT – III (13 Hours)

Chemistry of p-Block Elements

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, catenation, allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behavior of first member of each group. interhalogen and pseudohalogen compounds, Structure, bonding and properties (acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat) of the following:

Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15, Group 16 and Group 17.

Oxides: oxides of phosphorus, sulphur and chlorine

Oxoacids: oxoacids of phosphorus and chlorine; peroxyacids of sulphur

Halides: halides of silicon and phosphorus

UNIT – IV (10 Hours)

Noble gases

Occurrence and uses, rationalization of inertness of noble gases, clathrates; preparation and properties of XeF_2 , XeF_4 and XeF_6 . Molecular shapes of noble gas compounds (VSEPR theory).

Inorganic polymer

Preparation, properties, structure and uses of the following compounds: Borazine, Silicates, silicones, phosphonitrilic halides $\{(\text{PNCl}_2)_n \text{ where } n = 3 \text{ and } 4\}$, and concept of carbophosphazene.

Lab Work

(Credit-01)

(C L P = 1 0 1; Total Hours = $15 \times 2 = 30$)

(Laboratory periods: 30 Hours, 15 classes of 2 hours each)

List of experiments

1. Standardization of sodium thiosulphate solution by standard $\text{K}_2\text{Cr}_2\text{O}_7$ solution.

2. Estimation of copper using standard sodium thiosulphate solution (Iodometrically).
3. Estimation of available chlorine in bleaching powder iodometrically.
4. Preparation of Cuprous chloride (Cu_2Cl_2)
5. Preparation of Manganese(III) phosphate ($\text{MnPO}_4 \cdot \text{H}_2\text{O}$)
6. Preparation of Lead chromate (PbCrO_4)

Core- I

(Paper-VI)

Chemistry of halogen, oxygen and sulphur containing organic compounds

Course Objectives:

To provide the knowledge on organic compounds containing halogen, alcohol, phenol, thiol, ether, thioether, aldehydes, ketones, carboxylic acids and its derivatives as functional groups. Further to know their preparation, properties and reactivity for developing the skills required for synthesizing a target molecule from a given molecule.

Course Outcomes:

1. Understanding on preparation, properties and reactions of haloalkanes, haloarenes, and organic compounds containing C,H,O and S functional groups.
2. Basic knowledge on various name reactions and their mechanisms involving substitution, addition, elimination and condensation.
3. Knowledge on functional group interconversion and synthetic applications of different organic compounds.
4. Knowledge on various functional group detection in organic compounds and preparation of derivatives of functional groups.

Syllabus

Lecture-Credit-03 (45 Hrs)

Unit-I:

Chemistry of Halogenated Hydrocarbons (10 hrs)

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – $\text{S}_\text{N}1$, $\text{S}_\text{N}2$ and $\text{S}_\text{N}i$ mechanisms with stereochemical aspects and effect of solvent and nucleophiles. substitution vs. elimination.

Aryl halides: Preparation, including preparation from diazonium salts, nucleophilic aromatic substitution; $\text{S}_\text{N}Ar$, Benzyne mechanism.

Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit-II:

Alcohols, Phenols, Ethers and Epoxides (11 hrs)

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer-Tiemann and Kolbe's-Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, Ammonia derivatives and LiAlH₄.

Sulphur containing compounds: Preparation and reactions of thiols and thioethers

Unit-III:

Carbonyl Compounds (12 hrs)

Structure, reactivity and preparation. Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Perkin, Cannizzaro and Wittig reaction, Beckmann rearrangements, α halo-form reaction and Baeyer-Villiger oxidation, - substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, LiAlH₄, NaBH₄, MPVO.; Addition reactions of unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethylaceto acetate.

Unit-IV: Carboxylic Acids and Derivatives (12 hrs)

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic, lactic, malic, tartaric, citric, maleic and fumaric acids;

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann-bromamide degradation and Curtius rearrangement.

LAB WORK- Credit-01 (15 classes of 2 hours each)

List of Experiments

- 1. Functional group tests for amines (p-, sec- tert-), nitro, amide and imide groups in known organic compounds.**
- 2. Benzoylation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p- anisidine) and one of the following phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.**
- 3. Bromination of any one of the following:**
- 4. Acetanilide by conventional methods**

5.Acetanilide using green approach (Bromate-bromide method)

6.Nitration of any one of the following:

7.Acetanilide/nitrobenzene by conventional method

8.Salicylic acid by green approach (using ceric ammonium nitrate).

9.Identification of unknown organic compounds containing one functional group in CHO or CHN systems and their derivative preparation.

CORE-I PAPER-VII

Phase equilibrium, Chemical dynamics, catalysis and surface chemistry

Course Objectives:

This course is offered by School of Chemistry as a core subject for the B.Sc. programme, with an emphasis on fundamental understanding phase equilibrium and chemical kinetics. The objective of this course is to develop basic and advance concepts regarding of Surface chemistry and catalysis. It aims to study the similarity and differences between adsorption isotherms and reasons responsible for these. The objective of the practical is to develop skills for working in physical chemistry laboratory pertaining to kinetics & adsorption isotherms. The student will perform experiments based on the concepts learnt in Physical chemistry-III course.

Course Outcomes:

By the end of the course, the students will be able to:

- Establish the phase rule for one, two component systems, eutectics; and its thermodynamic derivation; fundamentals of physical transformation of pure materials.
- Interpret chemical kinetics of chemical reactions and its impact on reaction mechanism.
- Differentiate between homogenous and heterogenous catalysis & Acid Base Catalysis, differentiate between Physical adsorption, chemisorption and various adsorption isotherms.
- Determine distribution coefficients of solution mixtures, Interpret and use data generated from kinetic studies by graphical and experimental methods.

SYLLABUS

Lecture-Credit 03 (45 hours)

UNIT-I: Phase Equilibria-I (10 hr)

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications (H₂O and sulphur system). Phase diagrams for systems of solid-liquid equilibria involving eutectic (Pb-Ag system, desilverisation of lead), congruent (ferric chloride-water) and incongruent (sodium sulphate- water) melting points.

UNIT-II: Phase Equilibria-II (13 hr)

Three component systems, water-chloroform-acetic acid system, triangular plots.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), azeotropes, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst distribution law: its derivation and applications.

UNIT-III : Chemical Kinetics (12 hr)

Order and molecularity of a reaction, derivation of rate laws (Zero, first, and second order) and its differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of orders. Kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions (HBr chain reaction).

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, qualitative treatment of the theory of absolute reaction rates.

UNIT-IV Catalysis (10 hr)

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis- Menten mechanism, acid-base catalysis. Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms (Langmuir, Freundlich and Gibb's isotherms), nature of adsorbed state.

LAB WORK- credit 01 (15 classes of 2 hours each)

List of experiments

Determination of distribution coefficients of: Iodine between water and carbon tetrachloride.

Acetic/ benzoic acid between water and cyclohexane.

Study the equilibrium of at least one of the following reactions by the distribution

Method:

- $I_2(aq) + I^- \rightarrow I_3^-(aq)$
- $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n$
- Study the kinetics of the following reactions.

Integrated rate method: Acid hydrolysis of methyl acetate with hydrochloric acid.

Saponification of ethyl acetate.

Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.

Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

CORE-I PAPER-VIII

Coordination Chemistry, Chemistry of d- and f-block elements, Inorganic Reaction Mechanism and electron transfer reactions

Course Objectives:

To provide the knowledge on the coordination compounds which find manifold applications in the diverse fields such as industrial catalysis, metallurgy, pharmaceutical industry, paints and pigments. Students will achieve the knowledge about the diverse kinetic aspects of the coordination compounds. They will also be familiarized with the chemistry of d- and f-block elements and get an idea about horizontal similarity in a period in addition to vertical similarity in a group. Besides, the idea of inorganic reaction mechanism and the importance of electron transfer reactions have been reviewed. Synthesis and estimation of inorganic compounds have been included to enhance the practical skill of students in this regard.

Course Outcomes:

- Understand the chemistry of coordination compounds, and d- and f-Block elements.
- Explain magnetic properties and colour of complexes on the basis of Crystal Field Theory.
- Understanding the fundamental importance of inorganic reaction mechanism and electron transfer reaction
- Achieved the knowledge of the preparation of inorganic complex, estimation by EDTA method and gravimetric method.

SYLLABUS

(C L P = 3 3 0; Total Hours = 15 x 3 = 45)

UNIT – I (13 Hours)

Coordination Chemistry

Werner's Coordination theory, IUPAC nomenclature of coordination compounds, isomerism in coordination compounds with coordination numbers 4 and 6. A brief idea about chelate effect, and labile and inert complexes. Valence bond theory and its application to complexes of coordination numbers 4 and 6. Examples of inner and outer orbital complexes. Crystal field theory and its application, measurement of Δ_o . Calculation of CFSE in weak and strong fields, concept of pairing energies, factors affecting the magnitude of Δ_o . Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry, Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field theory, and MO Theory (bonding and antibonding interactions, idea about σ , σ^* , π , π^* , n -MO).

Synthesis of hexamine nickel(II) complex, $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$

Synthesis of tetraamminecopper(II) sulphate, $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

Estimation of Ca and Mg from cement by EDTA method

Estimation of nickel (II) using dimethylglyoxime (DMG)

UNIT – II (13 Hours)

Chemistry of d- and f-Block Elements

Chemistry of transition metals: General group trends with special reference to electronic configuration, colour, variable valency, magnetic properties (no temperature dependence), catalytic properties, and ability to form complexes. Distinction among the first, second and third transition series. Chemistry of Ti, V, Cr, Mn, Fe and Co in various oxidation states (excluding their metallurgy). Some important compounds of Cr, Mn, Fe and Co and their roles as laboratory reagents; Potassium dichromate, potassium permanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite. Chemistry of Lanthanides and Actinides: electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanide contraction (causes and effects), separation of lanthanides by ion exchange method. General features of actinides, separation of Np, Pm, Am from U.

UNIT – III (11 Hours)

Inorganic Reaction Mechanism

Thermodynamic and kinetic stability, Stepwise and overall formation constants and their relationship, factors affecting stability, Substitution reactions in square planar complexes, trans-effect, theories of trans-effect (electrostatic polarization and π -bonding theory), Substitution reactions in octahedral complexes, acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, test of conjugate base mechanism, anation reaction.

UNIT – IV (8 Hours)

Electron transfer reaction

Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non-complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.

Lab Work

Credit-01

(C L P = 1 0 1; Total Hours = $15 \times 2 = 30$)

(Laboratory periods: 30 Hours, 15 classes of 2 hours each)

List of experiments

- 1.Synthesis of hexamine nickel(II) complex, $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
- 2.Synthesis of tetraamminecopper(II) sulphate, $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$
- 3.Estimation of Ca and Mg from cement by EDTA method
- 4.Estimation of nickel (II) using dimethylglyoxime (DMG)

Core- I (Paper-IX)

Natural Products, Heterocyclic Compounds, Nitrogen containing compounds and Polynuclear Hydrocarbons

Course Objectives:

Imparting information on natural products, nitrogen based organic compounds, heterocyclic compounds and polynuclear hydrocarbons with their chemical properties and structural elucidation. Imparting hands on training in estimation and analysis of organic compounds.

Course Outcomes:

- Gaining knowledge on preparation, properties and synthetic application of nitrogen containing compounds including diazonium salts.
- Understanding on isolation and structural elucidation of natural products and heterocyclic compounds and their chemical reactions.
- Knowledge on structure and properties of fused aromatic compounds.
- Learning on various procedures of estimation of organic compounds.

SYLLABUS

Lecture-Credit-03 (45 Hrs)

Unit-I:

Nitrogen Containing Functional Groups (13 hrs)

Amines: Effect of substituent and solvent on basicity; Preparation from nitro and nitriles and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid.

Diazonium Salts: Preparation and their synthetic applications.

Unit-II:

Dyes and Polynuclear hydrocarbon derivatives (8 hrs)

Classification, colour and constitution; Mordant and Vat dyes; Chemistry of dyeing. Synthesis and applications of: *Azo dyes* – Methyl orange and Congo red (mechanism of Diazo coupling); *Triphenylmethane dyes*- Malachite Green, and crystal violet; *Phthalein dyes*– Phenolphthalein and Fluorescein. Edible dyes with example.

Preparation of Polynuclear Hydrocarbons: Reactions of naphthalene, anthracene, phenanthrene, acenaphthene, pyrene. Preparation and their structure elucidation (naphthalene) and important derivatives of naphthalene and anthracene.

Unit-III:

Heterocyclic Compounds (13 hrs)

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom, Reaction and mechanism of substitution reactions of: Furan, Pyrrole, Thiophene and Pyridine. Synthesis of Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis), Furan (Paal Knorr synthesis, Fieser-Benary Synthesis), Derivatives of Furan: Furfural and Furoic acid (preparation only) Pyridine (Hantzsch synthesis). Pyrimidine (synthesis from β -keto acid), Bicyclic Heterocyclic compound: Indole (Fischer indole synthesis and Madelung synthesis) Quinoline (Skraup synthesis, Friedlander Synthesis).

Unit-IV:

Natural Products (11 hrs)

Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action. Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation, synthesis and medicinal importance of Hygrine, Nicotine, Quinine and Morphine

Terpenes

Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, and α -terpineol.

LAB WORK

Credit-01 (15 classes of 2 hours each)

List of Experiments

- 1) Qualitative analysis of unknown organic compounds containing bifunctional groups
- 2) Estimation of Phenol/ Aniline
- 3) Estimation of Methyl Ketone
- 4) Determination of percentage purity of carbonyl compound.

CORE-I PAPER-X

Conductance, electrochemistry, electrical properties of atoms and molecules

The text provides an in-depth analysis of the conductance nature of electrolytic solutions, their thermodynamics, Debye-Huckel theory, ionic strength, mean ionic activity coefficient, and the Debye-Huckel limiting law.

Explain dynamic electrochemical processes and skill development to analyse it.

Understand the dynamic electrochemical processes and skill development to analyse it.

Develop skill to solve problems on Electrochemical Cells, electrode potentials, emf & solubility product measurements, potentiometric titrations, pK and pH measurements.

Course Objectives:

This course offers in introductory knowledge of electrolytic conductance depth knowledge of electrochemical cells. Students are expected to have background knowledge in physical chemistry and mathematics up to the +2 level for this course. The objective of the practical is to develop skills for working in physical chemistry laboratory. The student will perform experiments based on the concepts learnt in Physical chemistry-IV course.

Course Outcomes:

By the end of the course, the students will be able to:

- 1.The text provides an in-depth analysis of the conductance nature of electrolytic solutions, their thermodynamics, Debye-Huckel theory, ionic strength, mean ionic activity coefficient, and the Debye-Huckel limiting law.
- 2.Explain dynamic electrochemical processes and skill development to analyse it.
- 3.Understand the dynamic electrochemical processes and skill development to analyse it.
- 4.Develop skill to solve problems on Electrochemical Cells, electrode potentials, emf & solubility product measurements, potentiometric titrations, pK and pH measurements.

SYLLABUS

Lecture-Credit 03 (45 hours)

UNIT-I : Conductance-I (10 hr)

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

UNIT-II : Conductance-II (15 hr)

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

UNIT-III Electrochemistry-I (10 hr)

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry.

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application

to different kinds of half-cells. Application of EMF measurements in determining free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass electrodes.

UNIT-IV Electrochemistry-II (10 hr)

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). **Electrical properties of atoms and molecules:** Basic ideas of electrostatics, Electrostatics of dielectric media. Clausius-Mosotti equation and Lorenz-Laurentz equation (no derivation), Dipole moment and molecular polarizabilities and their measurements.

LAB WORK- credit 01 (15 classes of 2 hours each)

List of experiments

- I Determination of cell constant.
- II Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

Perform the following conductometric titrations: Strong acid vs. strong base

Weak acid vs. strong base

Strong acid vs. weak base

I Perform the following potentiometric titrations:

- i Strong acid vs. strong base
- ii Weak acid vs. strong base
- iii Dibasic acid vs. strong base

Core- I (Paper-XI)

Organic Spectroscopy

Course Objectives:

To provide knowledge on the principles of different advanced spectroscopic methods such as UV-Visible, FTIR, NMR and Mass-spectrometry and to develop analytical aptitude for interpretation of structure of the organic compounds by applying these spectroscopic methods. Imparting practical knowledge on UV-visible spectroscopy and colour of compounds.

Course Outcomes:

1. Gaining knowledge on principle of UV-visible and Infrared Spectroscopic techniques.
2. Gaining knowledge on principle of NMR Spectroscopic techniques.
3. Gaining knowledge on principle of Mass Spectrometry techniques.
4. Understanding and interpretation of different spectra of organic molecules.

SYLLABUS

Lecture-Credit-03 (45 Hrs)

Unit-I:

UV-Visible Spectroscopy (11 hrs)

Types of electronic transitions, λ_{max} , Lambert-Beer's law and its limitations, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Instrumentation (brief idea only), Application of Woodward rules for calculation of λ_{max} for the following systems: α , β - unsaturated carbonyl compounds, acids and esters; Conjugated dienes, distinction between cis and trans isomers.

Unit-II:

FTIR Spectroscopy (9 hrs)

Fundamental and non-fundamental molecular vibrations; IR absorption positions of O and N containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in simple functional group analysis.

Unit-III:

NMR Spectroscopy (15 hrs)

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Equivalent and non-equivalent protons, Spin-spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics; Interpretation of NMR spectra of simple organic compounds. ^{13}C NMR spectroscopy, chemical shift values and interpretation of NMR spectra. preliminary idea on NMR of ^{15}N , ^{19}F , ^{31}P nuclei.

Unit-IV:

Mass Spectrometry (10 hrs)

Introduction, Basic principle, Fragmentation pattern, instrumentation, Determination of molecular formulae, molecular ions, Parent peak, Base peak, isotopic peak and metastable ion peak. Use of molecular fragmentation, McLafferty rearrangement, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)

Problems involving identification of organic compounds using UV, IR, NMR and Mass spectroscopy.

LAB WORK

Credit-01 (15 classes of 2 hours each)

List of Experiments

1) Determine the λ_{max} value and predict the effect of auxochrome and conjugation on λ_{max} for the following molecules e.g. salicylic acid, benzoic acid and *p*-amino benzoic acid, cinnamic

acid, nitrophenols and nitrobenzene (in neutral, acidic and alkaline medium) by using UV-visible Spectrophotometer.

2) Identification of labelled peaks in the ^1H NMR spectra of the known organic compounds and to explain their δ -values and splitting pattern on a supplied NMR spectra.

3) Identification of labelled peaks in the IR spectrum of a compound and to explain the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C $\equiv$ C, C $\equiv$ N) of a supplied spectra.

CORE-I PAPER-XII

Basic quantum chemistry, Molecular & electronic spectroscopy, and photochemistry

Course Objectives:

This course is offered by School of Chemistry as a core subject for the B.Sc. programme, with an emphasis on fundamental understanding of Quantum chemistry, molecular spectroscopy, and photochemistry. Students are expected to have background knowledge in mathematics up to the +2 level for this course. The objective of the practical is to develop skills for working in physical chemistry laboratory. The student will perform experiments based on the concepts learnt in Physical chemistry-V course.

Course outcomes:

By the end of the course, the students will be able to:

1. Understand the postulates of quantum mechanics. Construct the Schrödinger wave equations for 1-D box, 3-D box, Rigid rotor, and SHO and able to interpret the solution of Schrödinger equation.
2. Understand LCAO-MO compare with VBT of H_2 molecule. Apply the fundamentals of Quantum mechanics to interpret molecular spectroscopy.
3. Calculate quantum yield of photochemical reactions.
4. Interpret the data obtained from graphical methods of Lambert-Beer's law experiments and correlate with UV-Vis spectroscopy.

SYLLABUS

Lecture-Credit 03 (45 hours)

UNIT-I: Quantum Chemistry-I (10 hr)

Quantum mechanical operators, Postulates of quantum mechanics, Schrödinger equation and its application to particle in one-dimensional box (complete solution) - quantization of energy levels, zero-point energy, normalization of wave functions, probability distribution functions, nodal properties. Extension to three-dimensional boxes.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Rigid rotator model of rotation of diatomic molecule: Schrödinger equation, transformation to spherical polar coordinates. Derivation of rotational energy expression of diatomic molecule.

UNIT-II Chemical Bonding (15 hr)

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO- MO treatment of H_2^+ . Bonding and antibonding orbitals. Qualitative extension to H_2 . Comparison of LCAO-MO and VB

treatments of H_2 (only wave functions, detailed solution not required) and their limitations.

Localized and non-localized molecular orbitals treatment of triatomic (BeH_2 , H_2O) molecules.

UNIT-III: Molecular Spectroscopy-I (10 hr)

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

UNIT-IV: Molecular Spectroscopy-II (10 hr)

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. *Electronic spectroscopy:* Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation.

Photochemistry Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching, chemiluminescence.

LAB WORK

Credit 01 (15 classes of 2 hours each)

List of experiments

- Study of absorption spectra (visible range) of KMnO_4 and determine the λ_{max} value. Calculate the energies of the transitions in kJ mol^{-1} , cm^{-1} , and eV.
- Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration.
- Determine the dissociation constant of an indicator (phenolphthalein).
- Determine the concentration of HCl against 0.1 N Na OH spectrophotometrically.
- To find the strength of given ferric ammonium sulfate solution of (0.05 M) by using EDTA spectrophotometrically.
- To find out the strength of CuSO_4 solution by titrating with EDTA spectrophotometrically.
- To determine the concentration of Cu(II) and Fe(III) solution photometrically by titrating with EDTA.

CORE-I PAPER-XIII

Chemistry of Organometallic Compounds

Course Objectives

To provide the basic knowledge and cutting-edge developments in the field of organometallic chemistry. This includes the classification of organometallic compounds, the concept of hapticity and the 18-electron rule governing the stability of a wide variety of organometallic species. Specific organometallic compounds are studied in detail to understand the basic concepts. It familiarizes the versatility of phosphine/NHC ligands as well as metathesis reactions. It provides much fundamentals about the qualitative inorganic analysis having multiple radical mixtures.

Course Outcomes:

- Understand the basic concepts of organometallic compounds pertaining to their synthesis, structure and bonding
- Understand the mechanistic phenomena of organometallic based catalytic reactions
- Get knowledge on the versatility of phosphine/NHC ligands, and industrially important metathesis reactions.
- Understand and explain the basic principles of qualitative inorganic analysis

SYLLABUS

(C L P = 3 3 0; Total Hours = 15 x 3 = 45)

UNIT – I (12 Hours)**Organometallic Compounds-I**

Definition of organometallic compound, classifications, nature of metal-carbon bond, nomenclature, the 18-electron rule, Concept of hapticity of organic ligands. Metal carbonyls: electron counting of metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear metal carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: preparation and structure, evidence of synergic effect and comparison of synergic effect with that in carbonyls.

UNIT – II (11 Hours)**Organometallic Compounds-II**

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethyl aluminium in the polymerisation of ethene and propylene (Ziegler – Natta Catalyst). Ferrocene: preparation and reactions (acetylation, alkylation, metallation, Mannich condensation, nitration, halogenation, silylation, borylation, sulphonation), structure and aromaticity, comparison of aromaticity and reactivity with that of benzene. Fluxional molecules. Concept of coordinative unsaturation, oxidative addition, reductive elimination, insertion reaction, migratory insertion, intramolecular hydrogen transfer reaction, agostic interaction.

UNIT – III (12 Hours)**Organometallic Catalysis**

General idea of catalysis, turnover number (TON), turnover frequency (TOF), hydrogenation of alkenes using Wilkinson's catalyst, Tolman catalytic loop, hydroformylation of alkenes (using cobalt catalyst), enantioselective hydroformylation, wacker process, Monsanto acetic acid synthesis, Cativa process, hydrosilylation reactions, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction). Concept of Pd-catalyzed cross-coupling reactions.

UNIT – IV (10 Hours)**Neutral Spectator Ligands and Metathesis Reactions**

Steric and electronic structure of phosphine ligands, basicity of phosphine, monodentate and multidentate phosphines, cone angle, bite angle, N-heterocyclic carbenes (NHC), synthesis of NHC, alkene metathesis, mechanism of alkene metathesis, classification of metathesis reactions, significance of metathesis reactions.

Lab Work

(C L P = 1 0 1; Total Hours = 15 x 2 = 30)

(Laboratory periods: 30 Hours, 15 classes of 2 hours each)

Experiment

1. Qualitative analysis of mixtures containing 4 radicals (2 anions and 2 cations). Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO₃²⁻, NO₂⁻, S²⁻, SO₃²⁻, F⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, PO₄³⁻, NH₄⁺, K⁺, Pb²⁺, Cu²⁺, Cd²⁺, Bi³⁺, Sn²⁺, Sb³⁺, Fe³⁺, Al³⁺, Cr³⁺, Zn²⁺, Mn²⁺, Co²⁺, Ni²⁺, Ba²⁺, Sr²⁺, Ca²⁺, Mg²⁺.

Mixtures may contain one insoluble component (BaSO₄, SrSO₄, PbSO₄, CaF₂ or Al₂O₃) or

combination of interfering anions e.g., CO₃²⁻ and SO₃²⁻; NO₂⁻ and NO₃⁻; Cl⁻, Br⁻, I⁻; Br⁻ and I⁻; NO₃⁻, Br⁻, I⁻.

Core- I (Paper-XIV)

Chemistry of Biomolecules

Course Objectives:

The objective of this course is to familiarize the student with biomolecules such as carbohydrates, amino acids, proteins, peptides, lipids and enzymes. The student will comprehend the structure, nomenclature, and properties of various biomolecules and their functions in biological systems. It will also help the learners to build the concept of metabolism by studying the chemistry and energetics of biomolecules in biochemical reactions.

Course Outcomes

- Imparting knowledge on various biomolecules with their detailed classification, structure, nomenclature and functions.
- Understanding the chemistry and energetics of food to energy conversion in biological systems.
- Gaining knowledge on type of enzymes and their roles in metabolism of biomolecules in various biochemical reactions.
- Practically determine saponification value and iodine number of fat and oil and determine the reducing and non-reducing sugars by Benedict's reagent.

Syllabus

Lecture-Credit-03 (45 Hrs)

Unit-I:

Carbohydrate (13 hrs)

Occurrence, classification (mono-, di- and poly- saccharides), chemical structure, constitution and absolute configuration of glucose and fructose, epimers and anomers relationships, mutarotation, determination of ring size of glucose and fructose, Haworth projections and Fischer projection conformational structures, interconversions of aldoses and ketoses. Chemical properties of monosaccharides and Killiani-Fischer synthesis and Ruff degradation; Synthesis of Disaccharides –(Sucrose, Lactose and maltose) by condensation reactions.

Unit-II:

Amino Acids, Peptides, Proteins and Nucleic acids (11 hrs)

Amino acids: Classification, Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis.

Peptides: Classification, Determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups- Solid-phase synthesis.

Proteins: Structure of proteins, protein denaturation and renaturation.

Nucleic Acids: Components of nucleic acids, Nucleosides and nucleotides; Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Structure of polynucleotides.

Unit-III:

Lipids (12 hrs)

Introduction to oils and fats, common fatty acids present in oils and fats, role of lipids in our body, structure and classification, importance of omega-3 and omega-6 fatty acids and their sources. Physical and chemical properties of oils and fats, acid value, saponification value, iodine value, smoke point, flash point, fire point, and specific gravity. Chemical reactions of oil and fat, rancidity, conversion of oil to fat through hydrogenation, Baudouin test, Halphens test, Hexabromide test.

Unit-IV:

Enzymes (9 hrs)

Introduction to enzyme nomenclature, classification and characteristics. Salient features of active site of enzymes. Enzyme-substrate formation theory. Mechanism of enzyme action, factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action, enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive including allosteric inhibition).

LAB WORK

Credit-01 (15 classes of 2 hours each)

List of Experiments

- (1) Determination of Saponification value of supplied oil.
- (2) Determination of Iodine value of supplied oil.
- (3) Qualitative analysis of carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.
- (4) Quantitative estimation of sugars:
 - a) Estimation glucose by titration with Fehling's solution.
 - b) Estimation glucose and sucrose in a given mixture.
- (5) Estimation of glycine by Sorenson's formalin method.
- (6) Study of the titration curve of glycine

CORE-I, PAPER-XV

Solid and porous materials, and magnetochemistry and power cells

Course Objectives:

To provide the basic understanding about the solid and porous materials with their diverse applications. Students will learn fundamentals of magnetochemistry and molecular magnetism which will be helpful for their competitive examinations. Course is designed to develop a comprehensive technological understanding in different power cells.

Course Outcomes:

1. Learn about the different materials, including theory and methods for the development of new materials with desired properties.
2. Know how pores can influence the properties of materials
3. Demonstrate an increased knowledge and understanding of magnetochemistry with critical thought and achieve the ability to analyze magnetochemical studies and data
4. Explain the principles that underlie the ability of various power cells and develop new idea of constructing power cells

SYLLABUS

(C L P = 4 4 0; Total Hours = 15 x 4 = 60)

UNIT – I (20 Hours)

Inorganic Solid Materials

Silicate industry:

Glass: Glassy state and its properties, classification (silicate and nonsilicate glasses), Manufacture and processing of glass, composite armoured properties of the following types of glasses: soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, colored glass, photosensitive glass.

Ceramics: Manufacture and types of ceramics, high technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes, carbon nanotubes and carbon fibers.

Cement: Classification of cement, ingredients and their role, manufacture of the cement, and their setting process and quick setting cements.

UNIT – II (15 Hours)

Crystal Engineering and Principle of Designing Porous Materials

Inorganic crystal engineering and design principle of metal-organic frameworks and organic-inorganic hybrids. Principles of ICE in the design of porous materials, their understanding and characterizations using X-ray diffraction and thermal methods. Surface characterization and surface behavior of such porous materials with special reference to the gas/solvent vapors sorption. Some special applications of such materials like gas storage, gas/solvent separation, etc. Understanding of the structure-property relationship for the design of functional molecular material or molecular devices- philosophy and the terminologies.

UNIT – III (15 Hours)

Magnetochemistry

Magnetic Substances: Terminology related with magnetic properties, Classification, Cooperative Magnetism, Ferromagnetic substances and related aspects, Application of hard and soft ferromagnetic substances. Para-, ferro- and antiferro-magnetism: Temperature dependence of magnetic susceptibility, Curie's Law and Curie-Weiss Law, Pathways of ferro- and antiferromagnetism, magnetic properties of an electron, paramagnetism and thermal energy, Spin-orbit Coupling, Magnetic properties of compounds of d- and f-block elements: concentrated and dilute systems, Magnetically frustrated systems, single molecule magnet (SMM), single ion magnet (SIM), single chain magnet (SCM).

UNIT – IV (10 Hours)

Power cells

Primary and secondary batteries, Battery components and their role, characteristics of battery, working principles of following batteries: Pb-battery, Li-battery, solid state electrolyte battery, fuel cell, solar cell, polymer cell.

Multi-Disciplinary Course - SEMESTER-I

Paper-I: Environmental Chemistry (Chemistry)

Course Objectives:

The objectives of a course in environmental chemistry typically aim to provide students with a deep understanding of the chemical processes occurring in the environment and their impacts on ecosystems, human health, and the planet as a whole with a comprehensive understanding of the components and processes of environmental systems, including the atmosphere, hydrosphere, lithosphere, and biosphere, and their interactions. Investigation of the chemical composition of environmental compartments, including the atmosphere (air pollutants), hydrosphere (water pollutants), and lithosphere (soil pollutants), and the sources, fate, and transport of pollutants in these compartments. To examine the chemical properties and toxicological effects of environmental pollutants on ecosystems and human health, including acute and chronic toxicity, bioaccumulation, bio magnification, and risk assessment.

Course outcomes:

- Gain a comprehensive understanding of the chemical processes occurring in the environment, including the sources, fate, and transport of pollutants
- Develop analytical skills in environmental chemistry, and apply a range of analytical techniques for the detection, and characterization of environmental pollutants.
- Aware of global environmental issues and challenges such as climate change, pollution, biodiversity loss, and resource depletion.
- Apply the principles of environmental chemistry for mitigating environmental pollution, promoting environmental conservation, and contributing to the development of environmentally friendly technologies and policies.

UNIT I

Environment Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, Biogeochemical Cycles of C, N, P, S and O. Bio distribution of elements. Hydrosphere Chemical composition of water bodies- lakes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution-inorganic, organic, pesticide agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters- dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards, Analytical methods for measuring BOD, DO, COD, F, oils, metals (As, Cd, Cr, Hg, Pb, Se etc) residual chloride and chlorine demand. Purification and treatment of water.

UNIT II

Soils composition, micro and macro nutrients, pollution-fertilizers, pesticides, plastics and metals, waste treatment Atmosphere Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals,

chlorofluorohydrocarbons. Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

UNIT III

Industrial Pollution Cement, Sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

UNIT IV

Environmental Toxicology, Chemical solutions to environmental problems, biodegradability, principles of decomposition.