Model Curriculum for Three/Four Year Degree Course (With Multiple Entry /Exit Option)

Based on NEP-2020

Chemistry

Odisha State Higher Education Council, Bhubaneswar

Government of Odisha

Contents

1. **Structure and Regulation……..**

2. **Core Courses (*4 Credits each*)……**

3. **Multidisciplinary Courses…….**
   *(3 courses to be chosen from **baskets of Multidisciplinary** for Semester-I/II/III with 3 credits each)*

4. **Ability Enhancement Courses……..**
   (Odia and English are the compulsory courses under Semester-I/II respectively with 4 Credits each)

5. **Skill Enhancement Courses (SEC)……....**
   *(3 courses to be chosen from **baskets of SEC** for Semester-I/II/III respectively with 3 credits each)*

6. **Value Added Courses…….....**
   a. ***Environmental Studies and Disaster management compulsory under Semester-I with 3 Credits***
   b. *3 courses to be chosen from **baskets of VAC** for Semester-III/V/VI with 3 credits each*

b. Summer Vocational Course ……
(Students may opt for vocational courses after 2nd Semester and 4th Semester for Certificate Course or Diploma Course respectively with 4 credit each)

Core I **Semester -I**

Atomic Structure, Periodicity of Elements and Chemical Bonding

Course Outcomes:

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

Unit – I: 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: 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 Walls 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: Chemical bonding

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-Lande 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: Chemical bonding

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: CH_4, H_2O, NH_3, PCl_3, PCl_5, SF_6, ClF_3, I_3^-, BrF_2^+, PCl_6^- , ICl_2^-, ICl_4^- , NH_4^+, $PO_4^{3-}$and SO_4^{2-}. 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, Mo l e c u l a r orbital diagrams of homo- & hetero-diatomic molecules (N_2, O_2, C_2, B_2, F_2, CO, NO) and their ions. Calculation of bond order. Concept of bent rule.

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.

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.

Text Books:

- ✓ *B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vishal Publishing Co., 33rd Ed., 2017.*
- ✓ *A. J. Elias, The Chemistry of the p-Block Elements-Syntheses, Reactions and Applications, University Press (India) Pvt Ltd., 2009.*
- ✓ *G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons, 1989.*

Reference Books:

- ✓ *J. D. Lee, Concise Inorganic Chemistry, Wiley India, 2010.*
- ✓ *B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of InorganicChemistry, John Wiley & Sons, 1994.*
- ✓ *P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller, F. A. Armstrong, Shriver and Atkins Inorganic Chemistry, 5th Edition, Oxford University Press, 2010.*
- ✓ *P. Chndra, C. Gupta, Chemical Dynamics and Coordination chemistry, 1st Ed., 2022.*
- ✓ *A. K. Das, M. Das, Fundamental Concepts of Inorganic Chemistry, 1st Edition,Volume CBS Publishers & Distributors Pvt. Ltd., 2014.*
- ✓ *J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry-Principles of Structure and Reactivity, Pearson Education, 2009.*
- ✓ *D. C. Harris, C. A. Lucy, Quantitative Chemical Analysis, 9th Ed, Freeman and Company,2016.*

Core 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.

Unit–I: Basics of Organic Chemistry

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

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**

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

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.

List of Experiments

1. Detection of extra elements (N, Cl, Br, I and S) in organic compounds by Lassaigne's test.
2. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid groups in known organic compounds.
3. Separation and purification of any one component of following binary solid mixture (Benzoic acid/*p*-Toluidine; *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotolune/*p*- Anisidine) based on the solubility in common laboratory reagents/solvents like water (cold, hot), ethanol (cold, hot), dil. HCl, dil. NaOH, dil.$NaHCO_3$ etc.
4. Determination of melting point and boiling point of different organic compounds

Text Books:

- ✓ *R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th Ed., Pearson Education India, 2010.*
- ✓ *A. Bahl, B. S. Bahl, Advanced Organic Chemistry, 5th Ed., S. Chand, 2012.*
- ✓ *B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, 2003.*

Reference Books:

- ✓ *T. W. Graham Solomons, C. G. Fryhle, S. A. Snyder, Solomons' Organic Chemistry, Global Ed., Wiley, 2024.*
- ✓ *J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford Publisher, 2012.*
- ✓ *R. K. Bansal, Organic Reaction Mechanism, 3rd Ed., Tata McGraw-Hill Publications, 1998.*
- ✓ *D. Nasipuri, Stereochemistry of Organic compounds, 4th Ed., New Age International Publisher, 2020.*
- ✓ *P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Pearson Education, 2003.*
- ✓ *F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part-A and Part-B, 5th Ed., Springer 2007.*
- ✓ *N. K. Vishnoi, Advanced Practical Organic Chemistry, 3rd Ed., Vikas Publishing House, 2009.*
- ✓ *O. P. Agarwal, Advanced Practical Organic Chemistry, Krishna Prakashan, 2014.*
- ✓ *V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, Universities Press, 2004.*
- ✓ *H. T. Clarke, A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, 2021.*

Core III **Semester II**

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:

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

Unit-I: Gaseous state

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 behavior, 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**

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

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 powderpattern method. Analyses of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals (stoichiometric and non- stoichiometric).

Unit-IV: Ionic equilibria

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.

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.

Text Books:

- ✓ *P. W. Atkins, J. de Paula, Elements of Physical Chemistry, Oxford University Press, 6th Ed., 2006.*
- ✓ *G. W. Castellan Physical Chemistry 4thEdn. Narosa 2004.*
- ✓ *Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co., New Delhi 2011.*

Reference books:

- ✓ *Puri, Sharma & Pathania, Principles of Physical Chemistry, Vishal Publishing Co, 47th Edn., 2017.*
- ✓ *R. G., Mortimer Physical Chemistry, Elsevier (Academic Press), 3rd Ed, 2008.*
- ✓ *T. Engel & P. Reid Physical Chemistry, 3rd Ed. Pearson 2013*
- ✓ *Kapoor K. L., Text Book of Physical Chemistry, McGraw Hill, 3rd Edn. 2017*
- ✓ *Hrishikesh Chatterjee, Understanding PHYSICAL CHEMISTRY Through Theories and Problems, Nonlinear insights (opc) pvt. ltd. Publication division, 1st Ed., 2023.*

Core 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 ($\Delta H_{neutralization}$, $\Delta H_{hydration}$ & C_V) for chemical reactions using calorimeter.

Unit-I: Chemical thermodynamics

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

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

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 (vant 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

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.

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.

Text Books:

- ✓ *P. W. Atkins& J. de Paula, Elements of Physical Chemistry, Oxford University Press, 6th Ed., 2006.*
- ✓ *D. A. McQuarrie, & J. D Simon. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi 2004.*
- ✓ *K. L. Kapoor, Text Book of Physical Chemistry, Mac Grow Hill, 3rdEdn. 2017*
- ✓ *B. D. Khosla, V. C. Garg, & A. Gulati, Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi 2011.*

Reference Books:

- ✓ *T. Engel & P. Reid, Physical Chemistry 3rd Ed. Pearson 2013.*
- ✓ *S.C. Kheterpal Pradeep's Physical Chemistry, Vol. I & II, Pradeep Publications 2011.*
- ✓ *Puri, Sharma &Pathania, Principles of Physical Chemistry, Vishal Publishing Co, 47th Edn., 2017.*

Core V **Semester III**

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.

Unit – I: 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: 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: 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 pseudo halogen 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; per oxoacids of sulphur
- **Halides:** halides of silicon and phosphorus

Unit – IV: 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 $\{(PNCl_2)_n$ where n = 3 and 4$\}$, and concept of carbophosphazene.

List of experiments

1. Standardization of sodium thiosulphate solution by standard $K_2Cr_2O_7$ 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 ($MnPO_4.H_2O$)
6. Preparation of Lead chromate ($PbCrO_4$)

Text Books:

- ✓ *A. J. Elias, The Chemistry of the p-Block Elements-Syntheses, Reactions and Applications, University Press (India) Pvt Ltd., 2009.*
- ✓ *J. D. Lee, Concise Inorganic Chemistry Wiley India, 5th Edn., 2008.*
- ✓ *J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry – Principles of structure and reactivity, Pearson Education, 4th Ed. 2002.*

Reference Books:

- ✓ *A. K. Das, Fundamentals of Inorganic Chemistry, Vol. I, CBS Publications, 2nd Ed., 2010.*
- ✓ *S. Prakash, G. D. Tuli, S. K. Basu, R. D. Madan, Advanced Inorganic Chemistry, Vol. I, 7th Ed., S. Chand & Company Pvt. Ltd., 2021.*
- ✓ *Puri, Sharma, Kalia, Principles of Inorganic Chemistry, Vishal Publication Co., 33rd Ed., 2017.*
- ✓ *D. E. Shriver, P.W.Atkins, Inorganic Chemistry, Oxford University Press, 5th Ed., 2010.*
- ✓ *G. L. Miessler, P. J. Fischer, D. A. Tarr, Inorganic Chemistry, 5th Ed., Pearson, 2014.*
- ✓ *J. Mendham, Vogel's Quantitative Chemical Analysis, 6th Ed., Pearson, 2009.*
- ✓ *V. K. Ahluwalia, S. Dhingra, A. Gulati, College Practical Chemistry, University Press, 2005.*

Core 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.

Unit-I: Chemistry of Halogenated Hydrocarbons

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – $SN1$, $SN2$ and SNi mechanisms with stereochemical aspects and effect of solvent and nucleophiles. substitution vs. elimination.
Aryl halides: Preparation, including preparation from diazonium salts, nucleophilic aromatic substitution; SNAr, Benzyne mechanism.
Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit-II: Alcohols, Phenols, Ethers and Epoxides

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

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

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.

List of Experiments

1. Functional group tests for amines (*p-*, *sec- tert-*), nitro, amide and imide groups in known organic compounds.
2. Benzolyation 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:
   a) Acetanilide by conventional methods
   b) Acetanilide using green approach (Bromate-bromide method)
4. Nitration of any one of the following:
   a) Acetanilide/nitrobenzene by conventional method
   b) Salicylic acid by green approach (using ceric ammonium nitrate).
5. Identification of unknown organic compounds containing one functional group in CHO or CHN systems and their derivative preparation.

Text Books:

- ✓ *R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th Ed., Pearson Education India, 2010.*
- ✓ *A. Bahl, B. S. Bahl, Advanced Organic Chemistry, 5th Ed., S. Chand, 2012.*
- ✓ *N. K. Vishnoi, Advanced Practical Organic Chemistry, 3rd Ed., Vikas Publishing House, 2009.*

  - *Reference Books:*

- ✓ *T. W. Graham Solomons, C. G. Fryhle, S. A. Snyder, Solomons' Organic Chemistry, Global Ed., Wiley, 2024.*
- ✓ *J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford Publisher, 2012.*
- ✓ *R. K. Bansal, Organic Reaction Mechanism, 3rd Ed., Tata McGraw-Hill Publications, 1998.*
- ✓ *P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Pearson Education, 2003.*
- ✓ *F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part-A and Part-B, 5th Ed., Springer 2007.*
- ✓ *B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, 2003.*
- ✓ *O. P. Agarwal, Advanced Practical Organic Chemistry, Krishna Prakashan, 2014.*
- ✓ *V. K. Ahluwalia, R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, Universities Press, 2004.*
- ✓ *H. T. Clarke, A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, 2021.*

Core 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:

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

Unit-I: Phase Equilibria-I

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 (H_2O 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

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

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

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.

List of experiments

1. Determination of distribution coefficients of:
   (a) Iodine between water and carbon tetrachloride.
   (b) Acetic/ benzoic acid between water and cyclohexane.
2. Study the equilibrium of at least one of the following reactions by the distribution method:

- $I_2\ (aq) + I^- \rightarrow I_3^-(aq)$
- $Cu^{2+}(aq) + nNH_3 \rightarrow Cu\ (NH_3)_n$

3. Study the kinetics of the following reactions.
   (i) Integrated rate method:
   a) Acid hydrolysis of methyl acetate with hydrochloric acid.
   b) Saponification of ethyl acetate.
   (ii) Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.
4. Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Text Books:

- ✓ *P. W. Atkins, J. de Paula, Elements of Physical Chemistry, Oxford University Press, 6th Ed., 2006.*
- ✓ *K. J. Laidler, Chemical kinetics, New York: Harper & Row 1916*
- ✓ *J. Rajaram, J. C. Kuriacose Kinetics and Mechanisms of Chemical Transformations, Penguin Books Ltd, 2000.*

Reference Books:

- ✓ *T. Engel, P. Reid, Physical Chemistry 3rd Ed. Pearson 2013.*
- ✓ *D. A. McQuarrie, J. D. Simon, Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi 2004.*
- ✓ *K. L. Kapoor, Text Book of Physical Chemistry, Mac Grow Hill, 3rdEdn. 2017*

Core VIII **Semester IV**

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 periodin 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 compoundshave been included to enhance the practical skill of students in this regard.

Course Outcomes:

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

Unit – I: 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).

Unit – II: 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 importantcompounds of Cr, Mn, Fe and Co and their roles as laboratory reagents; Potassium dichromate, potassiumpermanganate, 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: 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: 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.

List of experiments

1. Synthesis of hexamine nickel (II) complex, [Ni (NH3)6] Cl2
2. Synthesis of tetraamminecopper (II) sulphate, [Cu (NH3)4] SO4.H2O
3. Estimation of Ca and Mg from cement by EDTA method
4. Estimation of nickel (II) using dimethylglyoxime (DMG)

Text Books:

- ✓ *J. D. Lee, Concise Inorganic Chemistry, Wiley India, 5th Edn., 2008.*
- ✓ *J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry– Principles of structure and reactivity, Pearson Education, 4th Ed. 2002.*
- ✓ *F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry Wiley-VCH., 1999.*

Reference books:

- ✓ *A. K. Das, Fundamentals of Inorganic Chemistry, Vol. II, CBS Publications, 2nd Ed. 2010.*
- ✓ *G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons, 1989.*
- ✓ *Puri, Sharma, Kalia, Principles of Inorganic Chemistry, Vishal Pub. Co., 33rd ed., 2017.*
- ✓ *D. E. Shriver, P. W. Atkins, Inorganic Chemistry, Oxford University Press, 5th Edn.*
- ✓ *V. K. Ahluwalia, S. Dhingra, A. Gulati, College Practical Chemistry, University Press (2005).*
- ✓ *S. Gulati, J. L. Sharma, S. Manocha, Practical Inorganic Chemistry, 1st Edn., CBS Publishers & Distributors Pvt Ltd., (2017).*

Core-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:

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

Unit-I: Nitrogen Containing Functional Groups

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 Salt*s**:** Preparation and their synthetic applications.

Unit-II: Dyes and Polynuclear hydrocarbon derivatives

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

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, Fiest-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.

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.

Text Books:

- ✓ *R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th Ed., Pearson Education India, 2010.*
- ✓ *I. L. Finar, Organic Chemistry, Vol-2, 5th Ed., Pearson Publisher, 2002.*
- ✓ *N. K. Vishnoi, Advanced Practical Organic Chemistry, 3rd Ed., Vikas Publishing House, 2009.*

Reference Books:

- ✓ *T. W. Graham Solomons, C. G. Fryhle, S. A. Snyder, Solomons' Organic Chemistry, Global Ed., Wiley, 2024.*
- ✓ *J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford Publisher, 2012.*
- ✓ *J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th Ed., Wiley Blackwell, 2010.*
- ✓ *R. K. Bansal, Heterocyclic Chemistry, 5th Ed., New Age International, 2017.*
- ✓ *O. P. Agarwal, Organic Chemistry: Natural Products, Vol. I, Krishna Prakashan Media, 2015.*
- ✓ *H. T. Clarke, A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers, 2021.*

Core X

Conductance, electrochemistry, electrical properties of atoms and molecules

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.

Unit-I: Conductance-I

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

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

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

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.

List of experiments

I. Determination of cell constant.

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

III. Perform the following conductometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. 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

Text Books:

- ✓ *P. W Atkins. & J. de Paula, Elements of Physical Chemistry, Oxford University Press, 6th Ed., 2006.*
- ✓ *J. O. Bockris & A. Reddy. Modern Electrochemistry, Kluwer Academic, 2002.*
- ✓ *S. Glasstone, An Introduction to Electrochemistry: Affiliated East West Press Private, Limited. 1960*

Reference Books:

- ✓ *T. Engel & P. Reid, Physical Chemistry 3rd Ed. Pearson 2013.*
- ✓ *McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi 2004.*
- ✓ *Kheterpal S.C., Pradeep's Physical Chemistry, Vol. I & II, Pradeep Publications. 2002.*

Core XI **Semester V**

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.

Unit-I: UV-Visible Spectroscopy

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

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

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

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.

List of Experiments

1) Using an UV-visible spectrophotometer, obtain the uv-visible spectrum, determine the λ_{max} value and, after comparing the spectra of the following molecules, predict the effect of auxochrome and conjugation on absorption maxima.

   (a) Take and analyze the spectra of benzene, aniline, and 4-methoxyaniline using a suitable solvent. Then, compare the results after adding dil hydrochloric acid to it.

   (b) Take and analyze the spectra of salicylic acid, benzoic acid and *p*-amino benzoic acid, cinnamic acid in neutral and then compare the result after adding dil NaOH to it.

   (c) Take and analyze the spectra of o-nitrophenol, p-nitrophenols and nitrobenzene in neutral and then compare the result after adding dil NaOH to it.

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

2) 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≡C, C≡N) of a supplied spectrum.

Text Books:

- ✓ *W. Kemp, Organic Spectroscopy, 2nd Ed., Macmillan, 2019.*
- ✓ *P. S. Kalsi, Spectroscopy of Organic Compounds, 9th Ed., New Age International Publishers, 2022.*
- ✓ *D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy, 5th Ed., Cengage India Private Limited, 2015.*

Reference Books:

- ✓ Y. R. Sharma, Elementary Organic Spectroscopy, 5th Ed., S. Chand, 2013.
- ✓ Jag Mohan, Organic Spectroscopy: Principles and Applications, 2nd Ed., Narosa Publishers, 2009.
- ✓ J. Singh, J Singh, Organic Spectroscopy: Principles, Problems and their Solutions, Pragati Prakashan, 2019.
- ✓ R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identification of Organic Compounds, 8th Ed., Wiley, 2022.

Core 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 H2 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 corelate with UV-Vis spectroscopy.

Unit-I: Quantum Chemistry-I

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

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

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

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.

List of experiments

1. 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.
2. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
3. Determine the dissociation constant of an indicator (phenolphthalein).
4. Determine the concentration of HCl against 0.1 N Na OH spectrophotometrically.
5. To find the strength of given ferric ammonium sulfate solution of (0.05 M) by using EDTA spectrophotometrically.
6. To find out the strength of $CuSO_4$ solution by titrating with EDTA spectrophotometrically.
7. To determine the concentration of Cu (II) and Fe (III) solution photometrically by titrating with EDTA.

Text Books:

- ✓ *D. A. McQuarrie, Quantum Chemistry, Viva Books, Indian Student Edition, Reprint, 2011*
- ✓ *R.K. Prasad, Quantum Chemistry, New Age International, 2006*
- ✓ *I. Levine, Quantum Chemistry, 7th Edition, Pearson, 2000*

Reference Books:

- ✓ T. Engel & P. Reid, Physical Chemistry 3rd Ed. Pearson 2013.
- ✓ D. A. McQuarrie, & J. D. Simon, Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi 2004.
- ✓ S.C. Kheterpal Pradeep's Physical Chemistry, Vol. I & II, Pradeep Publications. 2011.

Core 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:

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

Unit – I: 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: 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: 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 hydrofomylation, wacker process, mosanto 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: 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.

Lists of 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:
   CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, F^-, Cl^-, Br^-, I^-, NO_3^-, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}.
   Mixtures may contain one insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of interfering anions e.g., CO_3^{2-} and SO_3^{2-}; NO_2^- and NO_3^-; Cl^-, Br^-, I^-; $Br^-$and I^-; NO_3^-, Br^-, I^-.

Text Books:

- ✓ *B. D. Gupta, A. J. Elias, Basic Organometallic Chemistry, 2nd Edn., University Press (2013).*
- ✓ *R. C. Mehrotra, A. Singh, Organometallic Chemistry, New Age International Publishers, 2nd Edn, 2000.*
- ✓ *Vogel's Qualitative Inorganic Analysis, 7th Ed, Revised by G. Svehela, 4th Ed., Person, 2007.*

Reference Books:

- ✓ *A. K. Das, Fundamentals of Inorganic Chemistry, Vol. II, CBS Publications, 2nd Ed. 2010.*
- ✓ *D. E. Shriver, P. W. Atkins Inorganic Chemistry, Oxford University Press, 5th Edn.*
- ✓ *J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry – Principles of structure and reactivity,Pearson Education, 4th Ed. 2002.*
- ✓ *B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vishal Publishing Co., 33rd Ed., 2017.*
- ✓ *J. F. Hartwig, Organotransition Metal Chemistry: From Bonding to Catalysis, University ScienceBooks, 2010.*

Core XIV **Semester VI**

Analytical Methods of Chemistry

Course Objectives:

This course is offered by School of Chemistry as a core subject for both 4-year B.Sc. with and without research Programs, with an emphasis on analytical methods of chemistry. This course aims to impart skills, promotes employability, and entrepreneurships in broad domains such as Thermal industry, pharma, dyes & paints, coating, metal & metallurgical PSUs, research, and academic institutes. Instrumentation proficiency: Students should gain hands-on experience with analytical instrumentation commonly used in chemical analysis, such as spectrophotometers, chromatographs, and mass spectrometers. The aims are to provide a sound physical understanding of the principles of analytical chemistry and to show how these principles are applied in chemistry and related disciplines— especially in life sciences and environmental science.

Course Outcomes:

1. Perform calibration and standardization procedures to ensure the accuracy and precision of analytical measurements, adhering to established protocols and standards.
2. Apply a variety of analytical techniques, such as spectroscopy, chromatography,

electrochemistry, and titrimetry, to quantitatively and qualitatively analyze chemical substances.

3. Collect, analyze, and interpret experimental data accurately using appropriate statistical methods and error analysis techniques.
4. Develop critical thinking and problem-solving skills and Implement quality control and assurance practices, including the use of control charts and validation of analytical methods, to ensure the reliability and reproducibility of analytical results.

Unit I – Tools and Data Handling

Calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of data; F, Q and t test, rejection of data, and confidence intervals.

Unit II – Separation Techniques

Solvent Extraction: distribution Coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter-current distribution. - Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. -Column, ion exchange, paper, TLC & amp; HPTLC: techniques and application. - Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Unit III – Spectroscopic Techniques

Electromagnetic radiation, absorption, and emission of radiation – instrumentation: sources, monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

Unit IV – Thermal and Electroanalytical Techniques

Thermogravimetry: instrumentation and techniques, TGA curves, DTA and DSC, applications. Electrogravimetry, coulometry, voltammetry, polarography, conductometry, instrumentation, techniques and application.

Textbooks:

- ✓ *D. C. Harris, Quantitative Chemical Analysis, 4th Edn., W. H. Freeman, 1995.*
- ✓ *G. D. Christian & J. E. O'Reily, Instrumental Analysis, 2nd Edn., Allyn & Balon, 1986.*
- ✓ *Skoog, Holler and Crouch, Principles of Instrumental Analysis, Cengage Learning, 6th Indian Reprint 2017.*

Reference books

- ✓ *W. H. Hobert: Instrumental Methods of Analysis, 7th Ed., Wardsworth Publishing Company, Belmont, California, USA, 1988.*
- ✓ *O. Mikes, & R.A. Chalmes, Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London. 2001*
- ✓ *Pavia, Lamman, Kriz and Vyvyan, Introduction to Spectroscopy, Cengage Learning, 3rd Indian Reprint 2017.*

Core 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 cell

Unit – I

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 : 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 : 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: 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.

Text Books:

- ✓ *F. Gomez-Granados, J. C. Moreno-Pirajan, L. Giraldo-Gutierrez, Porous Materials: Theory and Its Application for Environmental Remediation (Engineering Materials), Springer Nature Switzerland AG; 1st Ed. 2021.*
- ✓ *R. L. Dutta, A. Syamal, Elements of magnetochemistry, 2nd Ed, Affiliated East-West Press Pvt. Ltd, 2010.*
- ✓ *J. N. Lalena, D. A. Cleary, O. B. M. H. Duparc, Principles of Inorganic Materials Design, 3rd Ed, Wiley, 2020.*

Reference Books:

- ✓ *C. N. R. Rao, K. Biswas, Essentials of Inorganic Materials Synthesis, John Wiley & Sons, Inc., 2015.*
- ✓ *C. Julien, A. Mauger, A. Vijh, K. Zaghib, Lithium Batteries: Science and Technology, Springer, 2015.*
- ✓ *C. S. Solanki, Solar Photovoltaic Technology and Systems: A Manual for Technicians, Trainers and Engineers, Prentice Hall India Learning Pvt. Ltd., 2013.*
- ✓ *D. Pavlov, Lead-Acid Batteries: Science and Technology, Elsevier Science, 2015.*
- ✓ *S. P. Jiang, Q. Li, Introduction to Fuel Cells: Electrochemistry and Materials, Springer, 2022.*
- ✓ *A. Ramanan, G. R. Desiraju, J. J. Vittal, Crystal Engineering: A Textbook, World Scientific Publishing Co. Pte. Ltd., 2011.*
- ✓ *A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 2013.*

Core XVI **Semester VII**

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

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

Unit-I: Carbohydrate

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

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

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

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).

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
(7) Separation and identification of amino acids by paper chromatography
(8) Separation of blue and orange dyes from methyl orange by paper chromatography
(9) Separation and identification of food dyes by paper chromatography
(10) Separation of two immiscible liquids by paper chromatography
(11) Separation of blue and yellow dyes using isopropanol by paper chromatography

Textbooks

- ✓ *D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry, 7th Ed., W. H. Freeman Co., 2017.*
- ✓ *J. L. Jain, S. Jain, N. Jain, Fundamentals of Biochemistry, S. Chand, 2016.*
- ✓ *E. J. Wood, Wilson and Walker Principle and Techniques of Practical Biochemistry, Cambridge University Press, 2009.*

Reference Books:

- ✓ *D. Das, Biochemistry, 14th Ed., Academic Publishers, 2015.*
- ✓ *A. V. S. S. Rao, A Textbook of Biochemistry, 9th Ed., UBS, 2002.*
- ✓ *R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry, 7th Ed., Pearson Education India,2010.*
- ✓ *G. P. Talwar, L. M. Srivastava, Textbook of Biochemistry and Human Biology,3rd Ed., Prentice HallIndia, 2002.*
- ✓ *J. M. Berg, J. L. Tymoczko, L. Stryer, Biochemistry, 6th Ed., W. H. Freeman, 2006.*
- ✓ *P. J. Kennelly, K. M. Botham, O. Mcguinness, V. W. Rodwell, P. A. Weil, Harper's IllustratedBiochemistry, 32nd Ed., Lange-McGraw-Hill, 2022.*
- ✓ *T. W. Graham Solomons, C. G. Fryhle, S. A. Snyder, Solomons' Organic Chemistry, Global Ed., Wiley,2024.*

Core XVII

Polymer Chemistry

Course Objectives:

This course is offered by School of Chemistry as a core subject for the 4-year B.Sc. Programme, with an emphasis on fundamental understanding of the type of bond in a polymer and rationally design the monomers for a given polymer. To describe various methods used for synthesizing polymers. To use analytical methods to characterize a polymer. To study the properties of polymers.

Course outcomes:

5. The learners will be able to classify the polymers based on nature, occurance, mode of synthesis, thermal properties etc.
6. To differentiate between methods and mechanism of polymerization process.
7. Calculate molecular weights of polymers and study the applications & properties.
8. The learners will be able to design the monomers for the preparation of polymers of interest, characterize and understand the properties polymers.

Unit-I: Introduction and history of polymeric materials:

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

Functionality and its importance: Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi- functional systems, Poly-functional systems.

Unit-II: Mechanism & Kinetics of Polymerization

Polymerization reactions – addition and condensation, mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques. **Crystallization and crystallinity:** Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Unit-III: Molecular weight of polymers and their determination

(M_n, M_w, M_v, M_z) by end group analysis, viscometry and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. Glass transition temperature (T_g) and its determination: WLFequation, outlines of factors affecting glass transition temperature (T_g).

Unit-IV: Properties of polymers

(physical, thermal and mechanical properties). Preparation, structure, properties and applications of the following polymers: polyolefins (polyethylene, polypropylene), polystyrene, polyvinyl chloride, polyvinyl acetate, polyacrylamide, fluoro polymers (Teflon), polyamides (nylon-6 and nylon 6,6). Thermosetting polymers - phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, conducting polymers (polyacetylene, polyaniline). Brief outline of biodegradable polymers.

List of experiments

1. Preparation of nylon-6,6 / Polyaniline
2. Preparations of phenol-formaldehyde resin-novalac / phenol-formaldehyde resin resold.
3. Preparation of urea-formaldehyde resin
4. Redox polymerization of acrylamide
5. Precipitation polymerization of acrylonitrile
6. Determination of molecular weight by viscometry:
   a. Polyacrylamide / Polystyrene
   b. (Polyvinyl pyrolidine (PVP)
7. Determination of acid value/saponification value of a resin.
8. Determination of hydroxyl number of a polymer using colorimetric method.
9. Estimation of the amount of HCHO in the given solution by sodium sulphite method
10. Analysis of some IR spectra of polymers – Identification of labelled peaks in IR spectra of known polymer.

Text Books:

- ✓ *V. R. Gowarikar, Jayadev Sreedhar, N. V. Viswanathan, Polymer Science 1st Edition, New Age International Publishers, 1986.*
- ✓ *Premamoy Ghosh, Polymer Science and Technology: Plastics, Rubber, Blends and Composites, 3rd Edition, McGraw Hill Education, 2010.*
- ✓ *P. Bahadur & N.V.Sastry, Principles of polymer science, Narosa Publishing house, New Delhi2002.*

Reference books

- ✓ *L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)*
- ✓ *Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)*
- ✓ *Seymour/Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).*
- ✓ *Nayak P.L., Polymer Chemistry, Kalyani Publisher (2017).*
- ✓ *Hundiwale G.D., Athawale V.D., Kapadi U.R. and Gite V. V., Experiments in Polymer Science, New Age Publications (2009).*

Core XVIII

Green Chemistry

Course Objectives:

Basic introduction and explaining goals of Green Chemistry. Limitations/Obstacles in the pursuit of the goals of Green Chemistry, Principles of Green Chemistry with their explanations and examples and special emphasis on Designing a Green Synthesis using these principles.

Course outcomes:

1. Discuss about the role of principles of green chemistry.
2. Explain the importance of green synthesis.
3. Interpret the knowledge of prevention of hazardous chemicals in reactions.
4. Evaluate the efficiency of green catalysts & interpret the use of biocatalysts.

Unit-I: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Principles of Green Chemistry and Designing a Chemical synthesis-I

Twelve principles of Green Chemistry. Explanations of principle with special emphasis on - Designing green synthesis processes: Prevention of Waste/ by-products; maximize the incorporation of the materials used in the process into the final products (Atom Economy) with reference to rearrangement, addition, substitution and elimination reactions; Prevention/ minimization of

hazardous/ toxic products; Designing safer chemicals; Use of safer solvents and auxiliaries (e.g. separating agent) - green solvents (supercritical CO_2, water, ionic liquids), solventless processes, immobilized solvents.

Unit-II: Principles of Green Chemistry and Designing a Chemical synthesis-II

Explanation of green chemistry principles with special emphasis on: Energy efficient processes for synthesis - use of microwaves and ultrasonic energy. Selection of starting materials (use of renewable feedstock); avoidance of unnecessary derivatization (e.g. blocking group, protection groups, deprotection); Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products use of chemically safer substances for prevention of chemical accidents, inherent safer design greener - alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol); real-time, in-process monitoring and control to prevent the formation of hazardous substances; development of green analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit-III: Examples of Green Synthesis/ Reactions and some real-world cases-I

Green Synthesis of the following compounds: adipic acid, catechol, methyl methacrylate, urethane, disodium iminodiacetate (alternative to Strecker synthesis), paracetamol, furfural.

Microwave assisted reactions: Applications to reactions (i) in water: Hofmann Elimination, hydrolysis (of benzyl chloride, methyl benzoate to benzoic acid), Oxidation (of toluene, alcohols); (ii) reactions in organic solvents: Diels-Alder reaction and Decarboxylation reaction.

Ultrasound assisted reactions: Applications to esterification, saponification, Simmons-Smith Reaction (Ultrasonic alternative to Iodine).

Unit-IV: Examples of Green Synthesis/ Reactions and some real-world cases-II

Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments; Designing of Environmentally safe marine antifoulant; Rightfit pigment: synthetic azopigments to replace toxic organic and
inorganic pigments; Synthesis of a compostable and widely applicable plastic (poly lactic acid) from corn; Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

Future Trends in Green Chemistry

Oxidizing and reducing reagents and catalysts; multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Green chemistry in sustainable development. (Bio-diesel, bio-ethanol and biogas).

List of experiments

1. Acetylation of primary amine (Aniline to N-phenylacetamide) using Zn dust.
2. Nitration of salicylic acid by green method (Using calcium nitrate and acetic acid).
3. Bromination of acetanilide using ceric ammonium nitrate/KBr.
4. Microwave assisted nitration of Phenols using $Cu(NO_3)_2$.
5. Detection of elements in organic compounds by green method (Sodium carbonate fusion)
6. Base catalyzed Aldol condensation (Synthesis of dibenzalpropanone)
7. Vitamin C clock reaction using vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch. Effect of concentration on clock reaction.
8. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
9. Diels Alder reaction in water: Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.
10. Preparation and characterization of nanoparticles (Cu,Ag) using plant extract.

Text Books:

- ✓ *P.T. Anastas & J.K. Warner, Green Chemistry- Theory and Practical, Oxford University Press 2000.*
- ✓ *V.K. Ahluwalia & M. Kidwai.: New Trends in Green Chemistry, Anamalaya Publishers, New Delhi 2004.*
- ✓ *V. Kumar An Introduction to Green Chemistry, Vishal Publishing Co., 2015.*

Reference Books:

- ✓ *A.S. Matlack. Introduction to Green Chemistry, Marcel Dekker 2001.*
- ✓ *A K. Das and M. Das, Environment Chemistry with Green Chemistry, Books and Allied (P) Ltd. 2010.*
- ✓ *R.K. Sharma, I.T. Sidhwani &, M.K Chaudhari. I.K. Green Chemistry Experiment:A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN978-93-81141-55-7, 2013.*

- ✓ ***E-Contents:*** *The supporting materials can be found on the* ***website of the Berkeley Center for Green Chemistry (http://bcgc.berkeley.edu/)****.*
- ✓ ***Case Study:*** *https://shorturl.at/cjuHI*

Core XIX

Oxidation, Reduction, Reagents, Rearrangements and Name Reactions

Unit-I: Oxidation Reactions

Oxidation of (a) alcohols to carbonyls by chromium, manganese, aluminium, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents, (b) alkenes to epoxides by peroxides/per acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to carbonyls with bond cleavage by Manganese, Osmium, Ruthenium and lead based oxidants and ozonolysis (d) alkenes to alcohols/carbonyls without bond cleavage, Wacker oxidation, selenium, chromium based allylic oxidation process.

Unit-II: Reduction Reactions

Reduction reactions (a) in heterogeneous medium by Palladium/Platinum/Rhodium/Nickel (Resenmund reduction) and in homogeneous medium (Wilkinson reaction). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na in liquid ammonia (Birch reduction), Sodium, Magnesium, Zinc, Titanium and Samarium. (c) Reduction by hydride transfer reagents: Aluminium alkoxide, Sodium borohydride ($NaBH_4$), di-isobutylaluminium hydride (DIBAL-H), Sodium cyanoborodydride, Lithium trialkylborohydride, reduction with hydrazine (Wolff-Kischner reduction), reduction with trialkyltinhydride.

Unit-III: Reagents in Organic Synthesis

Functionalized Grignard reagents, organozinc, organo-lithium, organocopper, organopalladium, lithium diisopropylamide (LDA), Dicyclohexylcarbodiimide (DCC), organosilicon, organoborane, organotin, crown ethers, Dichlorodicyano benzoquinone (DDQ), Osmium tetroxide, 1,3-Dithiane, Trimethyl silyl iodide, Tri-n-butyl tin hydride.

Unit-IV: Rearrangement and Name Reactions

Nature of migration and migratory aptitude of groups in rearrangements reaction, Wagner-Meerwein, Favorskii, Fries, Benzil-Benzilic acid, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Schmidt, Lossen, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement, Wolff, Stevens reaction.

Recommended Textbooks:

- ✓ S. N. Sanyal, Reactions, Rearrangements and Reagents, 4th Ed., Bharati Bhawan Publishers & Distributors, 2019.
- ✓ R. K. Bansal, Organic Reaction Mechanism, 3rd Ed., Tata McGraw-Hill Publications, 1998.
- ✓ R. K. Bansal, Synthetic Approaches in Organic Chemistry, Narosa Publishing House, India, 1996.

Reference Books:

- ✓ W. Carruthares, I. Coldham, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, 2015.
- ✓ F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part-A and Part-B, 5th Ed., Springer 2007.
- ✓ J. March, M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Ed., Wiley, 2013.
- ✓ I. L. Finar, Organic Chemistry, Vol-2, 5th Ed., Pearson Publisher, 2002.
- ✓ R. O. C. Norman, J. M. Coxon, Principle of Organic Synthesis, 3rd Ed., CRC Press, 2017.

Core XX **Semester VIII**

Quantum chemistry & Statistical Thermodynamics

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 approximation method encompassing Linear variation principle, perturbation theory.
2. Apply HMO to different conjugated systems.
3. Acquire a firm knowledge of statistical methods, Ensambles, and apply the concept of molecular partition functions to macroscopic systems.
4. Compare the thermodynamic properties of different statistics.

Unit-I:

Approximation Methods: The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

Unit-II:

Huckell theory of conjugated systems, Calculation of π-bond energy, delocalization energy, electronic & charge density calculation, and bond order. Applications to ethylene, butadiene, cyclopropanol radical, and cyclobutadiene.

Unit-III:

Fundamentals of Statistical methods, Starling's approximation, Statistical Thermodynamics: mathematical & thermodynamic probability. Maxwell Boltzman distribution between partition function. Types of Partition functions: translational, rotational, vibrational and electronic partition functions.

Unit-IV:

Types of Statistics- Bose-Einstein statistics, Maxwell-Boltzman, Fermi-Dirac statistics. Calculation of results of three types of statistics.

Text Books:

- ✓ *D. A. McQuarrie, Quantum Chemistry, Viva Books, Reprint, 2011, Indian Student Edition*
- ✓ *Statistical Thermodynamics: M. C. Gupta, New Age Pvt Publication*
- ✓ *Statistical Mechanics and Thermodynamics, C. Garrod, Oxford Univ. Press, New York.*

Reference Book:

- ✓ *Atkin's Physical Chemistry: P. W. Atkins, J. D. Paula, Oxford University Press*
- ✓ *Statistical Mechanics, D. A. McQuarrie, University Science Books, California.*
- ✓ *Statistical Mechanics - A Concise Introduction for Chemists B. Widom, Cambridge University Press*

Core XXI

Chemical group theory, electronic spectra of metal complexes, and nuclear chemistry

Course Objectives:

To provide basic knowledge on symmetry of molecules applied through mathematical group theory. Gives idea about the electronic transitions between d-orbitals, L-S coupling, qualitative Orgel diagrams for different d^n systems, selection rules for electronic spectral transitions, charge transfer phenomena, Nuclear chemistry has been introduced to inculcate students about the chemistry of inner core of atoms. Lab work has been designed for preparing key inorganic compounds and estimating important ingredients of day-to-day use in a product in order to make students competent in this regard.

Course Outcomes:

1. Learn a significant knowledge on formal group theory for understanding molecular spectroscopy.
2. Explore the fundamentals of electronic spectra of coordination complexes.
3. Understand the stability of nucleus and its reactions, and the applications of radioisotopes in different fields.
4. Achieve the knowledge on quantitative estimation of important ingredients in various commonly used products, and also get the synthetic skills of preparing key inorganic compounds

Unit – I: Fundamentals of group theory

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, group multiplication table, group generators, symmetry of platonic solids, conjugacy relation and classes, matrix representation of symmetry elements.

Unit – II: Character table and normal modes

Character of a representation, reducible and irreducible representation, Great orthogonality theorem (qualitative description only), properties of irreducible representation. Character table (explanation and significance), construction of character tables for C_{2v} and C_{3v} point groups, direct product, standard reduction formula, Normal modes for C_{2v} and C_{3v} molecules.

Unit – III: Electronic spectra of metal complexes

Electronic transitions between d-orbitals, L-S coupling, Orgel diagrams for $3d^1$ to $3d^9$ ions. Selection rules for electronic spectral transitions, relaxation in selection rules. spectrochemical series of ligands, nephelauxetic series, Evaluation of Dq, B and beta (β) parameters for the complex, charge transfer spectra (elementary idea). Significance of Tanabe-Sugano diagram.

Unit – IV: Nuclear Chemistry

Nuclear stability, magic numbers, radioactivity, general characteristics of radioactive decay particles, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, nuclear cross section, compound nuclear theory, nuclear fission, liquid drop model, shell model, hard core preformation theory, fission fragments and their mass distribution, charge distribution, ionic charge of fission fragments, working principle of nuclear reactor, concept of boron-neutron capture therapy, concept of nuclear fusion.

List of experiments:

1. Estimation of iodine in iodized common salt iodometrically
2. Estimation of phosphoric acid in cola drinks by molybdenum blue method
3. Preparation of potash alum from scrap aluminum
4. Preparation of potassium of trioxalatoferrate (III) trihydrate, $K_3[Fe(C_2O_4)_3].3H_2O$
5. Determination of alkali content in antacid tablet using HCl
6. Determination of acetic acid in commercial vinegar

Text Books:

- ✓ *K. V. Ready, Symmetry and Spectroscopy of Molecules, New Age Int. Publishers, 2nd Ed, 2009.*
- ✓ *H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Pvt. Ltd., 4th Ed. 2011.*
- ✓ *A. Sakthivel , D. T. Masram, M. Sathiyendiran, S. Kaur-Ghumaan, Electronic and Magnetic Properties of Transition and Inner Transition Elements and Their Complexes, Publish with Nova Science Publishers, 2017.*

Reference Books:

- ✓ *F. A. Cotton, Chemical Applications of Group Theory, Wiley India (P) Ltd., 3rd Ed, 2009.*
- ✓ *G. L. Miessler, P. J. Fischer, D. A. Tarr, Inorganic chemistry, 5th Ed., 2014.*
- ✓ *D. E. Shriver, P. W. Atkins, Inorganic Chemistry, Oxford University Press, 5th Edn.*
- ✓ *D. Gabel, R. Moss, Boron Neutron Capture Therapy: Toward Clinical Trials of Glioma Treatment, Springer-Verlag New York Inc., 1st Ed, 2012.*
- ✓ *A. J. Elias, General Chemistry Experiments, University Press, 2007.*
- ✓ *Y. R. Sharma, Modern Approach to Practical Chemistry, Kalyani Publishers, 2008.*
- ✓ *Vogel's Qualitative Inorganic Analysis, 7th Ed, Revised by G. Svehela, 4th Ed., Person, 2007.*

Core XXII

Pericyclic reactions, Photochemistry and Retrosynthesis

Course Objective

Imparting knowledge in the theory and applications of various aspects of pericyclic reactions and photochemistry and synthetic aptitutde of organic molecules. It will also help to understand the synthesis and mechanisms of various reactions.

Course Outcome

1. Understand the concepts related to organic synthesis, mechanisms.
2. Apply their understanding about the photochemical reactions of industrial significance.
3. Evaluate the photochemical reactions based on the influence of the substituents on substrate
4. molecules.
5. Design new photochemical reactions in order to achieve the required product(s).

Unit-I: Pericyclic Reaction-I:

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams, FMO and PMO approaches. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Unit-II: Pericyclic Reaction-II:

Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems, Correlation diagrams and FMO method, Allowed and forbidden reactions. Diels-Alder reactions: retro Diels-Alder reaction- FMO mechanism for endo- and exo-selectivity, stereochemistry, inter- and intramolecular reactions.

Sigmatropic rearrangements: [i,j] H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations, Sommelet-Hauser, Claisen, thio-Claisen, Cope, Oxa and aza-Cope rearrangements, Ene reaction.

Unit-III: Photochemistry:

First order Photochemical processes Light absorption, Fluorescence and Phosphorescence. Photochemistry of Alkene: Isomerization, Intramolecular reactions of the olefinic bond,di-π-methane, oxa di-π- and aza di-π-methane rearrangements, Photochemistry of vision. Photochemistry of Carbonyl compounds: Norrish type I and II reaction, Paterno-Buchi reaction, Photoreduction. Photochemistry of Arenes: Photochemical aromatic substitution, addition and isomerisation reaction. Photo-Fries reactions of anilides, Barton reaction, the mechanisms of reactions involving free radicals- Sandmayer, Gomberg- Bachmann, Pschorr, Ulmann and Hunsdiecker reactions. Singlet molecular oxygen reactions.

Unit-IV: Retrosynthesis:

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis. one group C-X and two group C-X disconnections, chemo selectivity, reversal of polarity, cyclisation reactions. One Group C-C disconnection: Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. Two group C-C Disconnections:

Diels-Alder reaction, 1,3-difunctionalised compounds, α, β- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Michael addition and Robinson annulation. Protecting Groups, Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

List of Experiments

(1) Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
(2) Diels Alder reaction in water: Reaction between furan and maleic acid in water at room temperature rather than in benzene under reflux condition.
(3) Preparations of the following compounds: Aspirin/Paracetamol/Barbituric acid/
(4) Synthesis of methyl orange.
(5) Synthesis of amide derivative from carboxylic acid and amine or from esters
(6) Synthesis of esters by refluxing glacial acetic acid and ethanol in presence of sulphuric acid.
(7) Retrosynthetic analysis of biomolecules.

Textbooks

- ✓ *S. Warren, P. Wyatt, Organic synthesis, the disconnection approach, 2nd Ed., Wiley, 2012.*
- ✓ *J. Singh, J Singh, Photochemistry and Pericyclic Reactions, New Age Science, 2009.*
- ✓ *B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India, 2003.*

Reference Books:

- ✓ *S. Kumar, V. Kumar, S. P. Singh, Pericyclic Reactions: A Mechanistic and Problem-SolvingApproach, Academic Press, 2015.*
- ✓ *W. Carruthares, I. Coldham, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, 2015.*
- ✓ *J. March, M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Ed., Wiley, 2013.*
- ✓ *R. K. Bansal, Organic Reaction Mechanism, 3rd Ed., Tata McGraw-Hill Publications, 1998.*
- ✓ *R. K. Bansal, Synthetic Approaches in Organic Chemistry, Narosa Publishing House, India, 1996.*
- ✓ *J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford Publisher, 2012.*
- ✓ *T. L. Gilchrist, R. C. Storr, Organic Reactions and Orbital Symmetry, 2nd Ed., Cambridge University Press, 1979.*
- ✓ *F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part-A and Part-B, 5th Ed., Springer 2007.*
- ✓ *I. L. Finar, Organic Chemistry Vol. I & Vol. II, Longman, Cambridge, 2011.*

Core XXIII

Research Methodology for Chemistry

Course Objectives:

To make the students aware of fundamental but mandatory ethical practices in chemistry. chemistry. To introduce the concept of data analysis. To learn to perform literature survey in different modes. To make the students aware of safety handling and safe storage of chemicals. To make students aware about plagiarism and how to avoid it. To teach the use of different e-resources.

Course Outcomes:

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

1. Follow ethical practices in chemistry
2. Do Data analysis
3. Literature survey in different modes
4. Use e-resources.
5. Avoid plagiarism, understand the consequences and how to avoid

Unit-I: Scope of Research, Research Databases and Metrics

Define research problem, review literature, formulate hypothesis, design research/experiment, collect and analyse data, interpret and report, importance and future scope. **Print Database (traditional)**: Sources of information: Primary, secondary, tertiary sources; **Digital: Databases (modern source):** Google Scholar, Web of science, Scopus, UGC INFONET, SciFinder, PubMed, ResearchGate, E-consortium, e-books; **EBSCO:** e-Resources Gateway for Universities of Odisha (odisha university | OSHEC | e-Resources for Universities and Colleges of Odisha); **Research metrics**: Impact factor of Journal, h-index, i10 index, Altmetrics, Citation index; **Author identifiers/ profiles:** ORCID, Publons, Google Scholar, ResearchGate, VIDWAN.

Unit-II: Statistical tools and validation for chemists

Types of data, data collection-Methods and tools, data processing, hypothesis testing, Normal and Binomial distribution, tests of significance: t-test, F-test, chi- square test, ANOVA, multiple range test, regression and correlation. Features of data analysis with computers and softwares -Microsoft Excel, Origin, SPSS.

Unit-III: Research and Publication ethics:

Ethics with respect to science and research, Scientific Misconducts: falsification, fabrication and plagiarism, similarity index, software tools for finding plagiarism (Turnitin, Drillbit/Urkund etc), redundant publications; **Publication Ethics:** Introduction, COPE (Committee on Publication Ethics) guidelines; conflicts of interest, **publication misconduct:** problems that lead to unethical behaviour and vice versa, types, violation of publication ethics, authorship and contributorship, predatory publishers and journals; **IPR** - Intellectual property rights and patent law, commercialization, copy right, royalty, trade related aspects of intellectual property rights (TRIPS)

Unit-IV: Science Communications:

Types of scientific documents: Full length research paper, book chapters, reviews, short communication, project proposal, Letters to editor, and thesis; Thesis writing – Windows and/or linux operating system, programming fundamentals, basics of high level programming language-C: editing, compilation and running a programme, storing data, elementary numerical methods, different steps and software tools (Word processing, LaTeX, Chemdraw, Chemsketch etc) in the design and preparation of thesis, layout, structure (chapter plan) and language of typical reports, Illustrations and tables, bibliography, referencing: Styles (APA, Oxford etc), annotated bibliography, Citation management tools: Mendeley, Zotero and Endnote; footnotes; Oral presentation/posters – planning, software tools, creating and making effective presentation, use of visual aids, importance of effective communication, electronic manuscript submission, effective oral scientific communication and presentation skills.

Text Books:

- ✓ *Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow.*
- ✓ *Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry. Oxford University Press.*
- ✓ *Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.*

Reference Book:

- ✓ *Harris, D. C. Quantitative chemical analysis. 6th Ed., Freeman (2007) Chapters 3-5.*
- ✓ *Levie, R. de, how to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.*
- ✓ *Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992. OSU safety manual 1.01*

E-Contents:

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3. Web of Science
4. CAS Insights | CAS
5. Reveal online attention to research - Altmetric
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