PROPOSED SYLLABUS: CHEMICAL SCIENCES

1. Atomic Structure

- Basic principles of quantum chemistry: postulates; operator algebra; exactly solvable systems: particle-in-a-box, harmonic oscillator, rigid-rotor, and the hydrogen atom.
- Shapes of atomic orbitals; orbital and spin angular momenta; angular momentum operators, tunneling.
- Approximate methods of quantum mechanics: Variational principle; first-order perturbation. Many-electron systems and antisymmetry principle.

2. Molecular Structure and Bonding

- Chemical bonding; elementary concepts of molecular orbital (MO) and valence bond (VB) theories; Born Oppenheimer (BO) approximation, Hückel theory for conjugated π-electron systems. Valence bond (VB) theory.
- Molecular orbital (MO) theory: heteronuclear diatomic molecules, polyatomic molecules AH_n (n = 2 to 4).
- Ionic bond, covalent bond, metallic bond, coordinate covalent bond and weak chemical forces.

3. Nomenclature, Structure, and Isomerism of Organic Compounds

- Nomenclature, hybridization, resonance, frontier molecular orbitals, aromaticity, acidity and basicity, structure and stability of reactive intermediates (carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes).
- Isomerism, stereoisomerism (centre, axial, planar and helical chirality), configuration descriptors; topicity and descriptors; conformations of organic molecules.

4. Group Theory and Spectroscopy

- **Chemical applications of group theory:** symmetry elements; point groups; character tables; selection rules.
- **Atomic spectroscopy:** term symbols; **Molecular spectroscopy:** rotational, vibrational and Raman spectra; electronic spectra; basic principles of magnetic resonance.
- **Analytical Techniques for Inorganic Compounds:** Ultraviolet-Visible (UV-Vis) spectroscopy, fluorescence spectroscopy, Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy, nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy, mass spectrometry, cyclic voltammetry.
- **Interpretative Molecular Spectroscopy:** Structure elucidation of organic compounds using Fourier transform infrared spectroscopy (FTIR), ultraviolet-visible (UV-Vis), ^{1}H, ^{13}C nuclear magnetic resonance (NMR) and mass spectra. Determination of configurations and conformations and probing reaction mechanisms.

5. Chemical and Statistical Thermodynamics

- Laws of thermodynamics, state and path functions and their applications; thermochemistry, thermodynamic functions and their relationships; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; phase transitions, phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.
- Kinetic theory of gases; Boltzmann distribution; partition functions and their relation to thermodynamic quantities.

6. Electrochemistry

- Nernst equation, redox systems, electrochemical cells; Debye-Hückel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

7. Chemical Kinetics and Surface Chemistry

- Empirical rate laws and complex reactions; steady state approximation; mechanism of complex reactions, collision and transition state theories of rate constants; potential energy surfaces, unimolecular reactions, temperature dependence of rate constants; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions, fast reactions.
- Nuclear reaction processes. Kinetics of polymerization and molecular weight determination of polymers.
- Stability and properties of colloids; isotherms and surface area; principles of heterogeneous catalysis.

8. s and p Block Elements

- Periodic trends, hydrides, halides, oxides, oxoacids, nitrides, sulfides. Boranes, carboranes, silicones, silicates, boron nitrides, borazines and phosphazenes. Allotropes of carbon, phosphorous and sulphur. Noble gases.
- Acids and bases: Lewis, Brønsted, Hard and Soft Acids and Bases (HSAB). Nonaqueous solvent systems, liquid NH_3, liquid SO_2, superacids.

9. Properties and Reactions of Organic Compounds

- Synthesis and reactions of organic compounds: alkanes, alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines, amides, etc.
- Reactions of aromatic compounds: electrophilic and nucleophilic substitutions. Reagents for functional group interconversion, oxidation and reduction.
- Pericyclic reactions: cycloadditions, electrocyclic, sigmatropic, cheletropic and group-transfer reactions – stereochemical implications. Photochemical reactions.

10. d and f Block Elements

- **d-block elements and complexes:** Structure and isomerism of complexes. Periodic trends. Stability of various oxidation states. Crystal Field Theory (CFT) and Molecular Orbital Theory (MOT) of 4, 5, 6-coordinate complexes. Energy level diagrams, Crystal Field Stabilisation Theory (CFSE), applications of CFT, Jahn-Teller distortion. Metal-metal bonded compounds.
- **Spectroscopy and magnetism:** Term symbols, selection rules, Orgel and Tanabe-Sugano diagrams, spectrochemical series, nephelauxetic effect and Racah parameter, charge-transfer spectra. Magnetic properties.
- **Reaction mechanism:** Kinetic and thermodynamic stability, substitution. Electron transfer processes. Photochemistry of $[Ru(bpy)_3]^{2+}$ and related complexes.
- **f-block elements:** Electronic configuration, oxidation states, spectral and magnetic properties, Lanthanide contraction, separation of lanthanides.

11. Organometallic Compounds

- Synthesis, structure and bonding of organometallic compounds: metal-alkyl, carbene, alkylidene and alkylidyne, carbonyl, alkene and arene complexes and metallocenes. Fluxionality in organometallic complexes. Fundamental organometallic reactions.
- Homogeneous catalysis: hydrogenation, hydroformylation, acetic acid synthesis, metathesis, C-X bond forming reactions and olefin oxidation. Heterogeneous catalysis: Fischer-Tropsch reaction, Ziegler-Natta polymerization.

12. Bioinorganic Chemistry

- O_2: Evolution (Photosystem II), Carriers (Hb, Mb, Hr, Hc), Activation (Cytochrome P450, MMO) and Reduction (Cyt c oxidase).
- Electron transport (iron sulphur clusters, cytochromes, cofactors); hydrogenase and nitrogenase; Zinc containing enzymes.

13. Solid-state Chemistry and Inorganic Materials

- Crystal systems and lattices, X-ray crystallography, Miller planes, crystal packing, crystal defects, Bragg's law, ionic crystals, structures of AX, AX_2, ABX_3 type compounds, spinels, band theory, metals and semiconductors.

14. Reaction Mechanism

- Mechanisms of addition, elimination, substitution, condensation, concerted, rearrangement, fragmentation reactions. Generation and reactions of reactive intermediates. Common named reactions and their mechanism.
- Selectivity (chemo-, regio-, and stereo-selectivity) and stereo-electronic effects. Kinetic and thermodynamic control.

- Methods for probing reaction mechanisms – Hammond's postulate, reaction kinetics, Hammett equation, kinetic isotope effect, Curtin-Hammett principle.

15. Organic Synthesis

- Main group and transition metal-based reagents – formation of carbon-carbon single and multiple bonds. Applications of named reactions. Chemo, regio and stereo-selective transformations. Acid/base catalysis, organocatalysis, transition metal catalysed transformations.
- Retrosynthesis, disconnection, synthons, linear, convergent, divergent, diverted and iterative synthesis, umpolung, and protecting groups.
- **Asymmetric synthesis:** methods of asymmetric induction – substrate, auxiliary, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess. Resolution, kinetic, parallel and dynamic kinetic resolution, desymmetrisation. Specific examples of reactions – epoxidation, dihydroxylation, aldol, carbonyl addition, and hydrogenation.

16. Heterocyclic Chemistry

- Synthesis and reactivity of common heterocyclic compounds containing one or more heteroatoms (O, N, S). Chemistry of heterocycles in biological systems and pharmaceutical molecules.

17. Chemistry of Biological Molecules

- Structure, synthesis and reactions of amino acids, peptides, proteins, carbohydrates, fatty acids, nucleic acids and secondary metabolites (terpenes, alkaloids, polyketides, steroids, etc.) / natural products.

18. Data Analysis and Representation

- Precision and accuracy; significant digits, mean and standard deviation; absolute and relative errors; linear and non-linear regression, covariance and correlation coefficient. Linear, exponential, trigonometric and parabolic functions. Graphs.