Syllabus for PhD entrance exam-Chemistry

Section A: Inorganic Chemistry

Bonding - Ionic solids - Structures and energetics of metallic and ionic solids Solid Defects - Nonstoichiometric compounds -shapes of molecules (VSEPR Theory) - Molecular orbital theory of bonding – homo and heteronuclear molecules - General properties of elements - Chemical periodicity-

Acids, bases and ions in aqueous solution - Non-aqueous solvents – molten salts

s,p,d -block element chemistry - extraction-industrial applications – compounds, shapes, structures.

Chemistry of Halogens and Nobel gases - Inorganic cages-rings-clusters.

Coordination compounds: structure, isomerism, bonding theories, spectral and magnetic properties, reaction mechanisms. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.

The f-block metals: lanthanoids and actinoids

Organometallic compounds: synthesis, bonding and structure, and reactivity.

Catalysis and some industrial processes - Homogeneous and heterogeneous catalysis.

Nuclear chemistry - Detection of radioactivity, Decay processes, half-life of radioactive elements, fission and fusion processes.

Bioinorganic Chemistry: Ion (Na^+ and K^+) transport, oxygen binding, transport and utilization, photosystems, porphyrins, metalloenzymes, electron transfer reactions, nitrogen fixation, metalloenzymes containing magnesium, molybdenum, iron, cobalt, copper and zinc.

Physical techniques in inorganic chemistry - Characterization of inorganic compounds by IR, Raman, NMR, EPR, Mossbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.

Section B: Organic Chemistry

IUPAC nomenclature of organic molecules including Regio- and stereoisomers. Principles of stereochemistry - Determination of stereochemistry by spectroscopic methods - Stereoselective reactions of cyclic compounds – Diastereoselectivity.

Organic reaction mechanisms involving addition, elimination, and substitution reactions with electrophilic, nucleophilic or radical species – S_N1, S_N2, E1, E2, E1Cb – reactions, mechanism.

Determination of reaction pathways. Common named reactions and rearrangements - applications in organic synthesis.

Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic).

Concepts in organic synthesis: Retrosynthesis, disconnection, synthons. Asymmetric synthesis: Pericyclic reactions - electrocyclization, cycloaddition, sigmatropic rearrangements and other related concerted reactions.

Principles and applications of photochemical reactions in organic chemistry.

Structure determination of organic compounds by IR, UV-Vis, ^{1}H & ^{13}C NMR and Mass spectroscopic techniques.

Reaction Mechanisms: Basic mechanistic concepts - kinetic versus thermodynamic control, Hammond's postulate, and Curtin-Hammett principle.

Pericyclic reactions - cycloadditions - sigmatropic and electrocyclic reactions - Photochemistry of alkenes, arenes and carbonyl compounds. Photooxidation and photoreduction.

Reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals.

Uses of Mg, Li, Cu, B, Zn, P, S, Sn and Si based reagents in organic synthesis. Carbon-carbon bond formation through coupling reactions.

Heterocyclic compounds- Natural products - Polymerization.

Named reactions and rearrangements- Protection and deprotection of functional groups.

Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Concepts of multistep synthesis - retrosynthetic analysis, strategic disconnections, synthons and synthetic equivalents.

Conformations of Alkanes and Cycloalkanes – Stereochemistry - Nucleophilic Reactions - Alkenes and Alkynes - Alcohols and Ethers - Aldehydes and Ketones - Carboxylic Acids and Their Derivatives - Conjugated Unsaturated Systems – Amines-Aromatic Compounds - Reactions of Aromatic Compounds – Carbohydrates – Lipids - Amino Acids and Proteins - Nucleic Acids.

Experimental techniques in organic chemistry: Optical rotation. Applications of various chromatographic techniques such as thin-layer, column, HPLC and GC. Applications of UV-visible, IR, NMR and Mass spectrometry in the structural determination of organic molecules.

Section C: Physical Chemistry

The properties of gases – Laws of thermodynamics. Standard states. Thermochemistry. Thermodynamic functions and their relationships: Gibbs-Helmholtz and Maxwell relations, Gibbs-Duhem equation, van't Hoff equation. - Physical transformations of pure substances-Phase rule – Phase diagram.

Ideal and Non-ideal solutions, The properties of solutions – activity and activity coefficients -Raoult's Law and Henry's Law, Chemical equilibria – colligative properties of dilute solutions.

Standard electrode potentials and electrochemical cells. Nernst Equation and its application, relationship between Electrode potential and thermodynamic quantities, Potentiometric and conductometric titrations.

Statistical thermodynamics: microcanonical, canonical and grand canonical ensembles, Boltzmann distribution, partition functions and thermodynamic properties.

Molecular symmetry - Operations and symmetry elements -point groups - the symmetry classification of molecules.

Structure: Postulates of quantum mechanics. Operators. Time dependent and time independent Schrödinger equations. Born interpretation. Particle in a box: infinite and finite square wells; concept of tunnelling; particle in 1D, 2D and 3D-box; applications. Harmonic oscillator: harmonic and anharmonic potentials.

Rotational motion: Angular momentum operators, Rigid rotor. Hydrogen and hydrogen-like atoms : atomic orbitals; radial distribution function. Born- Oppenheimer approximation; Valence bond theory and linear combination of atomic orbitals – molecular orbital (LCAO-MO) theory. Hückel approximation and its application to annular π – electron systems.

Russell-Saunders coupling; Term symbols and spectral details.

Spectroscopy: Atomic spectroscopy; origin of selection rules. Molecular spectroscopy: rotational and vibrational spectra - electronic transitions- Rotational, vibrational, electronic and Raman spectroscopy of diatomic and polyatomic molecules. Line broadening. Basic principles of nuclear magnetic resonance: gyromagnetic ratio; chemical shift, nuclear coupling.

Kinetics -The rates of reactions- Integrated rate laws - Reactions approaching equilibrium - The temperature dependence of reaction rates- enzyme kinetics.

Potential energy surfaces, Transition state theory: Eyring equation, thermodynamic aspects. Kinetics of polymerization. Catalysis concepts and enzyme catalysis. heterogeneous catalysis – surface chemistry. Kinetic isotope effects. Fast reaction kinetics: relaxation and flow methods. Diffusion controlled reactions. Kinetics of photochemical and photophysical processes.

Solid state - Crystal lattices - lattice planes - Crystal structures- Bragg's law.

Section D: Analytical Chemistry

Errors in Chemical Analyses – Significant figures- Standard Deviation - Gravimetric Methods of Analysis - Titrations in Analytical Chemistry – Neutralisation titrations - Complexation and Precipitation Reactions and titrations –Oxidation/reduction titrations.

Electrochemical Methods- Standard Electrode Potentials - Oxidation/Reduction Titrations – Potentiometry - Electrogravimetry and Coulometry – Voltammetry.

Spectrochemical Analysis - Molecular Absorption Spectrometry - Molecular Fluorescence Spectroscopy- Atomic Spectroscopy- Mass Spectrometry.

Analytical Separations- Solvent extraction -Chromatography- Gas Chromatography- High-Performance Liquid Chromatography- LC/MS and GC/MS.

Miscellaneous:

Medicinal chemistry-Polymer chemistry-Nanoscience and technology-Supramolecular chemistry.