O P JINDAL UNIVERSITY
O P Jindal Knowledge Park, Punjipathra, Raigarh-496109
Department of Chemistry, School of Science

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 – SN1, SN2, 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– Neutralization 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.