



Chemistry Syllabus for PhD Entrance Test

Unit-I

Chemical Periodicity: Important periodic properties of the elements, covalent radii, ionic radii, ionization potential, electron affinity and electronegativity.

Bonding: Chemical bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory), MO Theory.

Concepts of Acids and Bases: Lux-Flood and solvent system concepts. Hard-soft acids and bases.

d-block and f-block Elements: General properties, comparison of 3d, 4d and 5d elements. Spectral and magnetic properties of compounds of actinides in comparison with those of lanthanides and d-block elements.

Coordination Compounds: Preparation of complex compounds, Stability of complex ions in solution, Coordination number and geometry, Bonding in coordination compounds, Electronic spectra and magnetic properties. Reactions of coordination compounds.

Organometallic Compounds: Fundamental concepts, Preparation, structure and bonding in metal carbonyls (nickel, cobalt, iron and manganese), nitrosyls, alkene and ferrocene.

Homogeneous and Heterogeneous Catalysis: Alkene hydrogenation, the Wacker process, Monsanto acetic acid process and water-gas shift reaction and Ziegler-Natta catalysis.

Unit-II

IUPAC nomenclature of organic compounds, **Structure and Reactivity:** Acids and bases, Structural effects on acidity and basicity, Hydrogen bonding, Resonance, Inductive and hyperconjugation effects, Concepts of aromaticity.

Reaction Intermediates: Carbocations, Carbanions, Free radicals, Carbenes, Nitrenes, Nitrogen, sulphur and phosphorous ylides.

Stereochemistry: Principles, Conformational analysis, Isomerism, Chirality.

Reaction Mechanisms: Mechanism of aliphatic and aromatic nucleophilic and electrophilic substitution reactions, Elimination reactions, Addition reactions and mechanisms of reactions of carboxylic acids and their derivatives.

Heterocyclic Chemistry: Synthesis, typical reactions and applications of 3-, 4-, 5-, 6- membered and fused ring systems.

Oxidation and Reduction: Oxidation with chromium and manganese compounds, Peroxides, Peracids, Lead tetraacetate, Periodic acid, OsO₄, SeO₂, NBS, Chloramine-T, Sommelet oxidation, Oppenauer oxidation; Catalytic hydrogenations, Wilkinson's catalyst, Baker's yeast, LiAlH₄, NaBH₄, Birch reduction, Leukart reaction, Hydroboration, Meerwein-Ponndorf-Verley reduction, Wolf-Kishner reduction, Clemenson reduction.

Molecular Rearrangements: involving carbon to carbon, carbon to nitrogen and miscellaneous rearrangements

Reagents: Gilmann reagent, DCC, DDQ, Crown ethers, LDA, Ziegler-Natta catalyst, Diazomethane, Stannous chloride, Sharpless epoxidation, Woodward and Prevost hydroxylation, Peterson reaction, Reformatsky reaction, dithiane, Wittig reaction.

Named Reactions: Mechanism and synthetic applications of aldol condensation, Claisen-Schmidt, Perkin, Cannizzaro's, Michael addition and Robinson's annulation reactions.

Unit-III

Electrochemistry: Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation, Debye-Huckel limiting law, Theories of electrical double layer, Concentration cells, Liquid junction potential, Over voltage, Conductometric and potentiometric titrations, Electrophoresis and zeta potential, True, apparent and abnormal transport numbers, Corrosion inhibition & prevention.

Chemical Kinetics: Arrhenius equation, Energy of activation & its determination, Order of reaction, parallel, consecutive & reversible reactions. Simple collision and activated complex theory, Effect of pressure on rates of reactions, Langmuir's theory of surface reactions. Experimental techniques of fast reaction kinetics, Chain reactions, Linear free energy relationship, Hammett & Taft equations, Swain-Scott and Edward equation.

Thermodynamics: Concept of entropy & free energy, Helmholtz and Gibbs free energies, Maxwell relations, Third law of thermodynamics, Partial molar properties, Chemical potential, Gibb's Duhem equation, Fugacity, Raoult's law & Henry's law, Heat capacity of solids, Phase rule & its applications, Principle of equipartition of energy, Relation between thermodynamic probability & entropy, Maxwell-Boltzman distribution equation, partition function.

Quantum Chemistry: deBroglie equation, Heisenberg Uncertainty principle, operators, Schrodinger wave equation for particles.

Nuclear Chemistry: Radioactive decay, Half life, Liquid drop nuclear model, Definition of curie, Magic number, alpha and beta decay, Binding energy, Oppenheimer-Phillips process, Spallation reactions, Bethe's notation, Nuclear reactions.

Crystallography: X-ray crystallography, Miller indices, Bragg equation, Powder and rotating crystal technique. Nano particle, nano wires and nano rods, Sol-gel and Chemical Vapour Deposition methods.

Unit-IV

Errors in Analytical Measurements: Measurement errors, absolute and relative error, determinate and indeterminate errors. Assessment of accuracy and precision. Significance testing-t-F-and Q-tests, Calibration and linear regression. Acid-base titrations - indicators and applications. Complexation, precipitation and redox titrations. Gravimetry - conditions of precipitation, co-precipitation and post-precipitation, PFHS, Organic precipitating agents, Examples of gravimetric analysis.

Potentiometric Electrodes and Potentiometry: Indicator and reference electrodes, glass pH electrode, Ion-selective electrodes, Solid-state ISFET electrodes, Direct potentiometry and potentiometric titrations.

Electrogravimetry: Effect of current on cell potential, Ohmic potentials; IR drop, Polarization effects. Electrogravimetric methods - Electrogravimetry without potential control, controlled potential electrogravimetry, Instrumentation and applications.

Thermal Methods of Analysis: Thermogravimetry, Differential thermal analysis and differential scanning calorimetry, Thermomechanical analysis, Evolved gas analysis and Thermometric titrations.

Atomic Spectrometric Methods: Flame emission spectrometry and Atomic absorption spectrometry.

Chromatography: Principles, Classification of chromatographic techniques, Theory of column efficiency in chromatography. Gas Chromatography: Performing GC separations, GC columns and detectors, temperature selection, Quantitative measurements, Headspace analysis, Thermal desorption, purging and trapping, GC-MS. Liquid Chromatography: HPLC - Principles, Stationary phases, Equipment for HPLC. HPLC method development, Fast liquid chromatography, LC-MS. Thin Layer Chromatography: Principles, methodology, instrumentation and applications. Capillary chromatography and Capillary gel electrophoresis.

Unit-V

Basic Concepts of Molecular Symmetry and Group Theory: Symmetry elements and symmetry operations, Correlation of Schoenflies and Hermann-Mauguin symbols for symmetry elements, Multiplication tables for the symmetry operations of simple molecules, Properties and definition of group theory, Point groups of simple molecules

Basic Principles and Application of Spectroscopy: Electromagnetic radiation, Types of molecular spectra.

UV-Vis Spectroscopy: Beer's law, Types of absorption bands ($n-\pi^*$, $\pi-\pi^*$, $n-\sigma^*$, $\sigma-\sigma^*$), Instrumentation (single and double beam), Qualitative and quantitative applications, Chromophores, Auxochromes, Solvent effect, Effect of polarity on various type of bonds, Predicting λ_{max} using Woodward's empirical rules of simple compounds.

IR Spectroscopy: Instrumentation of IR spectrometers (single and double beam), Characteristic group frequencies, Finger print region, Identification of functional groups, Tautomerism, Cis-trans isomerism, Applications.

Mass Spectroscopy: Principle, Instrumentation, Molecular ion, Base peak, Meta-stable peak, Nitrogen rule, McLafferty rearrangement, Mass spectral fragmentation of some simple organic compounds.

NMR Spectroscopy: Principle, Relaxation processes, Chemical shift and factors affecting it, Spin-spin coupling, Simplification of complex spectra, Contact shift reagents, Double resonance, NOE; ^{13}C NMR spectroscopy and its comparison with ^1H NMR, Multiplicity, Proton decoupling, Application of ^{13}C NMR, NMR of ^{19}F , ^{31}P , ^{11}B and ^{15}N . Composite problems involving UV-Vis, IR, NMR and mass for structural elucidation of simple organic compounds.