Bharath INSTITUTE OF HIGHER EDUCATION AND RESEARCH
(Declared as deemed to be university under section 3 of UGC Act 1956, vide notification No.F.9-5/2000-U.3)

Syllabus for Entrance Test for Ph.D. Admissions
Department of Chemistry

Physical and theoretical Chemistry

Atomic structure: Bohr's model – results of wave mechanical model – quantum numbers – shapes of orbitals.

Chemical kinetics and equilibrium: Rates of reactions – 1st and 2nd order reactions – activation energy – K_p, K_x, K_n, etc. – homogeneous chemical equilibria – acids and bases – pK_a of acid – solubility product.

Thermodynamics and thermo chemistry: Isothermal and adiabatic processes – carnot cycle, First, second and third laws of thermodynamics and their applications, entropy – free energy and chemical potential – chemical equilibria – phase equilibria, C_v and C_p, Hess law – Kirchoff's law – surface chemistry and thermodynamics – adsorption – solid state chemistry with reference to adsorption – solution chemistry – colligative properties – solvation – polar solvents.

Chemical Dynamics: Kinetic theory of gases – kinetics of reactions in the gas phase – theories of reactions – collision theory – transition state theory – applications of thermodynamic concepts to reactions – complex reactions such as parallel, consecutive and reversible reactions – chain reactions and their kinetics – kinetics in the liquid phase – effect of medium on reactions – homogeneous and heterogeneous catalysis – photochemistry in the gas phase and in solution – fluorescence – mechanism of photochemical reactions – irreversible processes in solution – fast reactions - viscosity – diffusion – sedimentation – behaviour of large molecules in solution – surfactants and their properties.

Electrochemistry: Conductance of electrolytes – transference – cells, half cells – Nernst equation – simple applications of conductivity and potentiometry Electrochemical cells – Nernst equation – theory of strong electrolytes (Debye-Huckel theory) – electrical double layer Lippman equation and structure – electrokinetic phenomena – basic electrode kinetics – Butler Volmer equation – Tafel equation – electroanalytical techniques (e.g polarography etc.)

Quantum chemistry and Chemical bonding: Schroedinger equation (SE) - postulates of quantum mechanics – operators – operators (Hamiltonian, angular momentum, spin and ladder) – exact solution of SE for some systems eg. Particle in the box, rigid rotor harmonic oscillator – approximate methods, variations and perturbation methods – LCAO – MO and VB methods. MO of diatomics and correlation diagrams – Huckel MO (HMO) theory and application to simple systems (eg. conjugated polyenes etc.) hybrid orbitals, molecular geometry.

Nuclear Chemistry: Nuclear reactions – fission and fusion – Radioactive decay process – interaction of radiation with matter.

Spectroscopy: UV-Vis, IR, Raman spectroscopy – principles of NMR and ESR spectroscopy – spin – spin splitting – hyperfine interactions – fundamental understanding of ESCA and Moss bauer spectroscopy - theories of the above spectroscopies with quantum mechanical approach – applications.

Inorganic and Analytical Chemistry

Analytical Chemistry: Principles of volumetric and gravimetric analysis, organic reagents in inorganic analysis, Principles of Instrumental methods in analysis – neutron activation, isotope solution analysis, spectrophotometry and flamephotometry, general applications of instrumental methods of chemical analysis – electrochemical and spectroscopic methods in analytical chemistry.

Chemistry of main group elements: A comparative account of the Chemistry of alkali, alkaline earth metals, non-transition elements and rare gases.

Solid State Chemistry: Crystal systems, Bravais crystal system, crystal symmetry, symmetry elements in a cubic system, laws of crystallography, atomic radius, number of atoms per unit cell, atomic packing factor, Weiss and Miller indices, interplanar spacing, X-ray studies of crystals-Bragg's equation, imperfections in crystals, structure of CsCl, CaF_2, TiO_2, diamond and graphite, Electronic properties of solids, band theory.

Synthetic Inorganic Chemistry: Synthesis, principles and structures of the following compounds, boron hydrides, boron anions, carboranes, compounds having B-N, B-P, Si-O, P-N, S-N, metal-hydrogen and metal carbon bonds – noble gas compounds.

Coordination compounds and transition metals: Coordination number – nomenclature – measurement of stability constants of complexes – mono and polyligated systems. Coordination components, isomerism, Principles of VB, MO and LF approaches, eleectronic spectrum and magnetic properties. Reaction mechanism of square planar and octahedral complexes. d_n configurations and their theoretical analysis R – S states – CF and LF theories – state splitting in different fields. Electronic spectra of complexes. Lanthanides – their properties – spectral and magnetic properties of lanthanides and transition and metal complexes.

Organo-Metallics: Metal carbonyls – olefin and acetylene complexes – metallocenes – haemoglobin.

Organic Chemistry

Reaction Mechanism: Chemical bonding and structure – nucleophilic substitution reactions at saturated carbon atoms – neighboring group participation – carbonium ion rearrangements – mechanisms of oxidation of alcohols and ketone reductions.
Elementary treatment of reaction of type S_N1, S_N2, E1 and E2. Hoffmann and Saytzeff Rules – substitutions at the aromatic ring, electrophilic, nucleophilic and radical – correlation of structure and reactivity – inductive, resonance and steric effects.

Reactions: Cycle additions – hydroboration – Hunsdiecker, Dieckmann, reactions, Cope, Fries and Claisen rearrangements and their mechanism – electron deficient carbon and nitrogen mediated rearrangements – Witting, Wolff, Hoffmann, Curtius, Schmidt rections – Mannich, Favorski, Michael, Robinson reactions – enolates and enamines.

Reagents used in organic synthesis (like $KMnO_4$, $K_2Cr_2O_7$, $LiAlH_4$, $NaBH_4$, Wilkinson's catalyst, DCC, etc.)

Organic Photo Chemistry: Reactions of carbonyl compounds – dienes, cycloadditions – Woodward –Hoffmann rules – applications.

Terpenes: Classification – syntheses – structural elucidation of mono terpenoid and diterpenoids.

Steriods: Classification – rearrangements of steroids – photo chemical transformations – Barton reaction – cholesterol – synthesis of aromatic steroids.

Structural Elucidation by Spectroscopic Methods: Application of UV, IR and NMR spectroscopy to structural analysis of organic compounds. IUPAC system of nomenclature, alkanes, alkenes, dienes, ketones, alcohols, amines and carboxylic cids – their preparation and properties. **Aromaticity** and benzene chemistry.

Stereo Chemistry: Optical activity – asymmetric synthesis – conformational analysis of cyclohexanes and decalines – octat rule. Cyclohexane – Conformational analysis geometric isomerism concepts of Z and E, R and S notations.

Heterocyclic compounds: Preparation, properties of Thiophene and pyrrole.