



K L UNIVERSITY

K L University, 29-36-38, Museum Road, Governorpet
VIJAYAWADA - 500 002,
Phone Number 08662577715, [http:// www.kluniversity.in](http://www.kluniversity.in)

Syllabus for Entrance Test for PhD Admissions Department of Chemistry

Section-1 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: Schrodinger 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.



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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.

Section-2 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 flame photometry, 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, CaF₂, TiO₂, 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, electronic spectrum and magnetic properties. Reaction mechanism of square planar and octahedral complexes. dⁿ 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.



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Section-3 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 – Wittig, Wolff, Hoffmann, Curtius, Schmidt reactions – 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.

Steroids: 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 acids – 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.