Syllabus for Ph.D Pre - Registration Qualifying Entrance Exam

Unit 1: Inorganic Chemistry

Chemical periodicity - Structure and bonding in homo and heteronuclear molecules, including shapes of molecules (VSEPR Theory) - Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents - Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds - Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms - Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications - Organometallic compounds: synthesis, bonding and structure, and reactivity - Organometallics in homogeneous catalysis - Cages and metal clusters - Analytical chemistry - separation, spectroscopic, electro- and thermoanalytical methods - Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron - transfer reactions; nitrogen fixation, metal complexes in medicine.

Unit II: Organic Chemistry

IUPAC nomenclature of organic molecules including regio and stereoisomers - Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction - Aromaticity: Benzenoid and nonbenzenoid compounds – generation and reactions - Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes - Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species - Determination of reaction pathways - Common named reactions and rearrangements and applications in organic synthesis - 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 in organic synthesis: Retrosynthesis, - Asymmetric synthesis - Pericyclic reactions - Principles and applications of photochemical reactions in organic chemistry - Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S) - Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids - Biogenesis of terpenoids and alkaloids -

Unit III: Physical Chemistry

Quantum chemistry: Postulates of quantum mechanics, wave functions and probabilities, Eigen functions and Eigen values, Schrodinger equations, John-teller effect, Pauli principle, Self-consistent field, atomicorbitals, Slater Type Orbitals - Group theory: Symmetry elements and symmetry operations Centre of symmetry, Plane and its types of Symmetry, Proper and Improper axis of Symmetry, Character Tables for C_{2V}. Mutual exclusion rule for molecules with center of symmetry, Selection rules forn-π^* and π-π^*

transitions in formaldehyde molecule - Chemical kinetics: Rate laws and rate constants, reaction order, determination of rate law, reactions approaching equilibrium, temperature dependence of reaction rates, Chain reactions and its rate laws, enzyme catalysis, catalytic efficiency of enzymes - Thermodynamics: First law of thermodynamics, Second law of thermodynamics, Carnot's principle, Gibbs and Helmholtz energies, The Maxwell relations, Concept of entropy, reversible and irreversible processes, Free energies, Fugacity - Photochemistry and surface chemistry: Photochemical laws, Quantum yield, electronically excited states, Jablonski diagram, Energy level diagrams, Fluorescence and Phosphorescence, Mechanism of energy transfer - Surface tension, solid-liquid interfaces; Physisorption and chemisorptions, Freundlich, Langmuir isotherms; Surface area determinations.

Unit IV: Spectroscopy Methods

UV-Visible spectroscopy - IR-Spectroscopy - Raman spectroscopy: Principles and applications of simple organic and inorganic molecules, predicting number of active modes of vibrations, analysis of representative spectra of metal complexes with various functional groups at the coordination sites; application of isotopic substitution - IR and Raman of H_2O, CO_2, N_2O, ClF_3, NO_3^-, ClO_4^- - ^1H NMR spectroscopy – origin – chemical shift, number of signals, peak area, multiplicity and coupling constants –^{13}C NMR spectra - Simplification of complex NMR spectra – Shift reagents – high fields – deutration – decoupling - Two dimensional NMR spectra – Applications of H-H COSY, C-H COSY, HMBC, INADEQUATE, DEPT and NOESY spectra - Multinuclear NMR of B, Al, Si, F and P nuclei; structure and dynamics of representative inorganic molecules - Electron paramagnetic resonance (EPR) spectroscopy of organic and inorganic compounds with unpaired electrons - determination of electronic structure, Zeeman splitting, g-values, hyperfine and super hyperfine coupling constants, practical considerations of measurements, and instrumentation - Mass spectrometry, basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, - Mossbauer effect, recoilless emission and absorption, hyperfine interaction, chemical isomer shift, magnetic hyperfine and quadruple interaction and interpretation of spectra -Fe, Sn.

Unit V: Nanochemistry and Green chemistry Applications

Chemistry in nanoscience and technology – Physicochemical methods-ball milling, electrodeposition, spray pyrolysis, flame pyrolysis, inert gas condensation technique, thermal evaporation, pulse laser deposition, C/RF magnetron sputtering, molecular beam epitoxy, sol-gel, self-assembly, solvothermal, photochemical, sonochemical, microemulsion, combustion, chemical vapour deposition, metal oxide chemical vapour deposition, metal nanocrystals by reduction and template process. Biological methods: protein-based, DNA-templated and lyotropic liquid crystal templated. characterisation of nanomaterials - Catalysis and green chemistry - Designing Green Synthesis: choice of starting materials, reagents, catalysts, biocatalysts, polymer supported catalysts, green solvents (water, ionic liquids, fluorous solvents, supercritical CO_2) - Synthesis involving principles of green chemistry - Renewable chemicals from biomass and sustainable polymers - Organic synthesis under microwaves: benefits, limitations, equipments. Ultrasound assisted reactions: esterification, reduction, coupling reactions. – Sensor applications - Solar energy conversion devices - photovoltaic cells - photoelectrochemical cells - semiconductor electrolyte junctions photocatalytic modes for fuel conversion process - photobiochemical options.