

Syllabus for Ph.D. CHEMISTRY Entrance Examination

10
note

I Research Methodology (50 %)

A. Basic tools & concepts for pursuing research

Importance of literature survey, planning a literature search, identifying key concepts and keywords, locating relevant literature and reliability of a source.

Science Citation Index–Journal Impact factors, h-index, g-index, i10 index, Chemical abstracts– UGC infonet, E-Journals and books–Search engines and databases

Ethics, moral philosophy, nature of moral judgements and reactions. Scientific conduct - ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts - falsification, fabrication and plagiarism. Redundant publications - duplicate and overlapping publications. Selective reporting and misrepresentation of data.

Best practices and standards, conflicts of interest, publication misconduct, unethical behaviour and related problems. Authorship and contributorship. Identification of publication misconduct, complaints and appeals.

Laboratory safety: Proper protection equipment - Fires, explosives and implosions - Extinguishing fires, explosions and implosions – Chemical spills on clothing and body, chemical Toxicity - First aid

B. Basic tools & concepts for pursuing research in Chemistry

Basic software tools for chemistry: MS office, Chemdraw, reference managers. Analytical methods and tools: Significant numbers, precision, accuracy and error bar. Solute, solvent and solution, concentration expressions (molarity, molality, normality, weight and volume percentages). Titrations – acid-base, redox, complex-metric, indicators, pH, Qualitative analysis of organic compounds, qualitative and quantitative analysis of inorganic ions (cations/anions). Principles and applications of UV-Vis, IR, Mass and NMR spectroscopic techniques.

C. Communication (Language) skills

Basic writing and reading comprehension skills in English (Part of Research Methodology)

II Chemistry (50 %)

Physical Chemistry: Atomic and Molecular Structure: Planck's black body radiation, Photoelectric effect, Bohr's theory, de Broglie postulate, Heisenberg's Uncertainty d and f orbitals; Pauli's Exclusion Principle; Hund's rule of maximum multiplicity; Schrödinger's wave equation, postulates of quantum mechanics, Shapes of s, p and d orbitals Gaseous State: Kinetic theory of gases: deviations from ideal gas behaviour. Liquid State: Physical properties of Liquid, vapour pressure and surface tension. Solid State: Unit Cells, Miller indices, crystal systems and Bravais Lattices, X-ray diffraction, Bragg's Law, Structure of NaCl, CsCl, KCl, CdI₂ and perovskite; different types of packing in solids, semiconductors, insulators; Defects in crystals, lattice energy; isomorphism; heat capacity of solids. Chemical Thermodynamics: Reversible and

irreversible processes; Laws of thermodynamics, thermochemistry, thermodynamic functions: enthalpy, entropy, and Gibbs free energy, their properties and applications; Partial molar quantities, dependence of thermodynamic parameters on composition, Gibbs Duhem equation and chemical potential. Chemical and Phase Equilibria: Law of mass action; K_p , K_c , K_x and K_n ; Effect of temperature on K ; Le-Chatelier principle; Ionic equilibria in solutions; pH and buffer solutions; Salt hydrolysis; Solubility and solubility product; Dilute solutions; Raoult's and Henry's Laws and their applications; Colligative properties; Gibbs phase rule; Electrochemistry: Conductivity, equivalent and molar conductivity and their properties; Kohlrausch law; Debye-Hückel-Onsager equation; Ionic velocities, mobilities, transference numbers; Applications of conductance measurement; Quantitative aspects of Faraday's laws of electrolysis. EMF of a cell, Nernst equation; Standard electrode potential, Electrochemical series; Concentration cells with and without transference; Applications of EMF measurements including potentiometric titrations. Chemical Kinetics: Order and molecularity of a reaction, rate expressions: differential and integrated form, type of reactions: opposing, parallel, and consecutive reactions; Steady state approximation, uni-molecular reaction; Temperature dependence of reaction rates, Arrhenius equation; activation energy; Collision theory of reaction rates; Types of catalysts, specificity and selectivity, Enzyme catalysis (Michaelis-Menten equation) Adsorption: Absorption and adsorption, adsorption isotherms; types of adsorption. Spectroscopy: Fundamental concepts of rotational, vibrational, electronic and magnetic resonance spectroscopy.

Organic Chemistry: Electronic effects (resonance, inductive, hyperconjugation) and steric effects and its applications (acid/base property); optical isomerism in compounds; conformation of acyclic systems (substituted ethane/n-propane/n-butane) and cyclic systems, substituted cyclohexanes, and polycyclic (cis and trans decalins) systems. E/Z and R/S configuration. Aromaticity and Hückel's rule, Organic Reaction Mechanism and Synthetic Applications: S_N1 , S_N2 , S_Ni , E1, E2, E1cB, Ei and neighboring group participation. Chemistry of reactive intermediates (carbocations, carbanions, benzyne); mechanisms of nucleophilic substitution and elimination reactions; Hofmann-Curtius-Lossen rearrangement, Wolff rearrangement, Reimer-Tiemann reaction, Michael reaction, Wittig reaction and McMurry reaction; Pinacol-pinacolone, Favorskii, benzylic acid rearrangement, Baeyer-Villiger reaction. Grignard, organolithium and organocopper reagents and applications; Diels-Alder reactions. Nomenclature of heterocyclic compounds with one and two heteroatoms (O, N and S). Structure and aromatic characteristics of pyrrole, furan, thiophene and pyridine; comparison of basicity of pyridine, piperidine and pyrrole Synthetic protocols and reactivity with particular focus on electrophilic substitution. Organic photochemistry and pericyclic reactions.

Inorganic Chemistry: Aufbau's principle, periodicity; effective nuclear charge, atomic, covalent, and ionic radii, ionization enthalpy, electron gain enthalpy, and electronegativity with atomic number, electronic configuration of diatomic molecules. Metallurgy: General methods of isolation and purification of elements; Principles and applications of Ellingham diagram. Chemical Bonding and shapes of molecules: Ionic

bond: Packing of ions in crystals, radius ratio rule, polarizing power and polarizability; Fajan's rules; Covalent bond: Lewis structure, valence bond theory. Hybridization, molecular orbital theory, molecular orbital diagrams of diatomic and simple polyatomic molecules ; Effect of intermolecular forces on melting and boiling points, bond dipole, dipole moment, and molecular polarizabilities; VSEPR theory and shapes of molecules. Main Group Elements (s and p blocks): Gradation of properties in a group; Inert pair effect; allotropes, structure and reactions of simple and industrially important compounds: boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes. Hydrides, oxides and oxoacids of pnictogens (N, P), chalcogens (S, Se & Te) and halogens, xenon compounds, pseudo halogens and interhalogen compounds; Symmetry: symmetry elements and point groups; General characteristics of d and f-block elements; coordination chemistry- structure and isomerism, stability, theories of metal-ligand bonding (CFT and LFT), mechanisms of substitution and electron transfer reactions of coordination complexes. Electronic spectra and magnetic properties of transition metal complexes, lanthanides and actinides. Metal carbonyls, metal-metal bonds and metal atom clusters, metallocenes; transition metal complexes with bonds to hydrogen, alkyls, alkenes and arenes; metal carbenes; use of organometallic compounds as catalysts in organic synthesis ; Organometallic compounds with metal-ligand single and multiple bonds (such as metal carbonyls, metal nitrosyls and metallocenes); Homogenous catalysis: Wilkinson's catalysis, Wacker's process, oxo process and Ziegler-Natta catalysis. The role of metal ions in biological systems, especially Fe. Structure and function of myoglobin and haemoglobin.

