

SYLLABUS FOR ENTRANCE TEST

Part – A Research Methodology

UNIT 1

Selection of research problems and literature survey; primary sources- Journals periodicals, abstracts; Secondary listing of titles, reviews – annual Treatise, serials, monographs and text book, encyclopedia, catalogues, index of tabulated data-science citation index- searching the chemical literature-location of journal article-materials on a given topic-information about specific compound-choosing a problem-abstract of a research paper.

Internet: Introduction to internet-web browsers-world wide web-search engines-literature survey in chemistry-popular website in chemistry-Database in chemistry.

E-mail: introduction to e-mail-creation of e-mail-Receiving and sending e-mail.

Patent: Introduction, patentable subject, steps involved in patenting.

UNIT 2

Purification of compounds; General Methods of isolation and purification of chemicals, Solvent extraction both cold and hot methods of crystallization, fractional crystallization, sublimation, Distillation; fractional distillation, distillation under reduced pressure, steam distillation, drying methods of solvents.

Handling of chemicals, hazardous chemicals air/water sensitive, corrosive, toxic, explosive, carcinogenic and radioactive materials.

Safety measures in laboratory, Good laboratory practices (GLP)

UNIT -3

Error Analysis in Chemical Measurements and results

Classification of errors-Accuracy-Precision-Minimization of errors-Significant figures. Statistical treatment of data: Mean and Standard Deviation-distribution of random and normal errors-Reliability of results-Confidence interval-Comparison of mean results students t-distribution and t-tests-Comparison of precision of two methods, comparison of precision of two methods- Linear regression, regression line, standard deviation, correlation coefficient-Multiple linear regression(one variable with two other variables).

Part – B Cognate Subjects

SECTION – I

Structure and Bonding: Atomic orbitals, electronic configuration of atoms (L-S coupling) and the periodic properties of elements; ionic radii, ionization potential, electron affinity, electronegativity; concept of hybridization. Shapes of polyatomic molecules; VSEPR, theory, symmetry elements and point groups for simple molecules. Bond lengths, bond angles, bond order and bond energies. Types of Chemical Bond (weak and strong) intermolecular forces, structure of simple ionic and covalent solids, lattice energy.

Acids and Bases: Bronsted and Lewis acids and bases, pH and pKa, acid-base concept in non-aqueous media; HSAB concept. Buffer solution.

Elementary principles and applications of electronic, vibrational, NMR, and Mass Spectral techniques to simple structural problems.

Topics in Analytical Chemistry: Solvent extraction and ion exchange, methods, Application of atomic and molecular absorption and emission spectroscopy in quantitative analysis. Electroanalytical techniques: Voltammetry, cyclic voltammetry, polarography, amperometry, coulometry and conductometry ion-selective electrodes. TGA, DTA, DSC – Elementary account.

SECTION – II

Chemistry of Non-transition Elements: Synthesis, properties and structure of boranes, carboranes, borazines, silicates phosphazenes, sulphur-nitrogen compounds. Rare gas compounds.

Chemistry of Transition Elements: Coordination chemistry of transition metal ions; Stability constants of complexes and their determination; Factors affecting stability of complexes. Stereochemistry of coordination compounds. CFT, splitting of d-orbitals, factors affecting and CFSE. Jahn-Teller effect; interpretation of electronic spectra including charge transfer spectra; spectrochemical series, nephelauxetic series Magnetism: Dia-, para-, ferro- and antiferromagnetism, quenching of orbital angular momentum, spin-orbit coupling, Inorganic reaction mechanisms; substitution reactions, trans effect and electron transfer reactions.

Chemistry of Lanthanides and Actinides: Spectral and magnetic properties; Use of lanthanide compounds as shift reagents in NMR.

Organometallic Chemistry of Transition Elements: Synthesis, structure and bonding, organometallic reagents in organic synthesis and in catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization); pi-acid metal complexes, metal carbonyls, sandwich compounds, Fluxional behavior of molecules.

Bioinorganic Chemistry: Metal ions in Biology, Molecular mechanism of ion transport across membranes; ionophores. Photosynthesis, PS-I, PS-II; nitrogen fixation, oxygen uptake proteins, Metallo enzymes (carbonic anhydrase, carbonic peptidase, Cu-Zn SOD).

SECTION – III

Separation Techniques

Chromatographic Techniques: Classification, basic principles, theory of chromatography.

Thin layer chromatography, paper chromatography, column chromatography, Ion exchange chromatography, High Performance liquid chromatography (HPLC)

Introduction, principle,

Instrumentation and applications. Gas chromatography: Characteristics of mobile, stationary phases used in GSC and GLC. Characteristics of carrier gases, detectors, application of GC-MS, LC-NMR, and MALDI-TOE

Common organic Reactions and Mechanisms: Reactive intermediates. Formation and stability of carbonium ions, carbanions, carbenes, nitrenes, radicals and arynes. Nucleophilic, electrophilic, radical substitution, addition and elimination reactions, Selective Organic Name Reactions: Aldol, Perkin, Stobbe, Dieckmann condensations; Reimer – Tiemann, Reformatsky and Grignard reactions. Diels-Alder reactions; Claisen rearrangements; Friedel – Crafts reactions; Wittig reactions; and Robinson annulation. Routine functional group transformations and interconversions of simple functionalities. Hydroboration, Oppenauer oxidations; Clemmensen, Wolff- Kishner, Meerwein-Ponndorf-Vereley and Birch reductions.: Favorski reaction; Michael addition, Mannich Reaction; Baeyer-Villiger reaction, Chichibabin reaction.

Rearrangements: Mechanism and applications of Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Wagner-Meerwein, Pinacol-Pinacolone, Favorskii, Curtius, and Benzil-Benzilic acid rearrangements.

Principles of organic synthesis: General planning – role of molecular starting materials and key intermediates.

Retro synthesis: Application of disconnection approach to the synthesis of atropine, citral, chloramphenicol, paracetamol, nicotine.

Reagents in organic synthesis: Complex metal hydrides, LDA, DDQ, Merrifield resins, 1,3-dithiane, selenium dioxide, Crown ethers – structure and their applications.

Aromaticity: Huckel's rule and concept of aromaticity annulenes and heteroannulenes, fullerenes (C₆₀).

Stereochemistry and conformational analysis:

Concept of Chirality: Recognition of symmetry elements and chiral structures; R – S nomenclature, diastereoisomerism in acyclic and cyclic systems; E-Z isomerisms.

Conformational analysis: Simple cyclic (chair and boat cyclohexanes) and acyclic systems. Interconversion of Fischer, Newman and Sawhorse projections.

Newer methods of asymmetric synthesis (including enzymatic and catalytic nexus), enantio and diastereo selective synthesis. Effects of conformation on reactivity in acyclic compounds and cyclohexanes.

Pericyclic Reactions: Selection rules and stereochemistry of electrocyclic reactions, cycloaddition and sigmatropic shifts, Sommelet, Hauser, Cope and Claisen rearrangements.

Heterocyclic Chemistry: Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fischer indole synthesis.

Bioorganic Chemistry: Synthesis of amino acids and peptides. Elementary structure and function of proteins and nucleic acids.

IR, UV-Visible, ¹H NMR and mass spectroscopy: Principle, instrumentation and applications- combined application of these in establishing the structure of compounds.

SECTION – IV

Quantum Chemistry: Planck's quantum theory, wave-particle duality. Uncertainty Principle, operators and commutation relations: postulates of quantum mechanics and Schrodinger equation; free particle, particle in a box degeneracy, harmonic oscillator, rigid rotator and the hydrogen atom.

Thermodynamics; First law of thermodynamics, relation between Cp and Cv; enthalpies of physical and chemical changes. Second Law of thermodynamics, entropy, Gibbs-Helmholtz equation. Third law of thermodynamics and calculation of entropy. Law of conservation of energy. Energy and enthalpy of reactions. Entropy, free-energy, relationship between free energy change of equilibrium.

Ideal and Non-ideal solutions. Excess functions, activities, concept of hydration number: activities in electrolytic solutions; mean ionic activity coefficient; Debye-Huckel treatment of dilute electrolyte solutions. Colligative properties: Vapour pressure, depression in freezing point, and elevation in boiling point.

Electrochemistry: Electrochemical cell reactions, Nernst equation, electrical double layer, electrode/electrolyte interface, Redox potential. Electrochemical series. Redox indicators, Batteries, primary and secondary batteries, Fuel cells, corrosion and corrosion prevention.

Surface Phenomena: Surface tension, adsorption on solids, electrical phenomena at interfaces, including electrokinetic, micelles and reverse micelles; solubilization, micro-emulsions.

Statistical Thermodynamics: Thermodynamic probability and entropy; Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Partition function: translational, vibrational and electronic partition functions for diatomic molecules; calculations of thermodynamic functions and equilibrium constants.

Reaction Kinetics: Order of a reaction (First, second and n^{th} order). Methods of determining rate laws, Mechanisms of photochemical, chain and oscillatory reactions. Collision theory of reaction rates; steric factor, treatment of unimolecular reactions. Theory of absolute reaction rates, comparison of results with Eyring and Arrhenius equations. Ionic reactions; salt effect. Homogeneous catalysis and Michaelis-Menten kinetics; heterogeneous catalysis. Luminescence and Energy transfer processes.

Macromolecules: Number-average and weight average molecular weights; determination of molecular weights, Kinetics of polymerization. Stereochemistry and mechanism of polymerization.

Nano materials: Introduction, Metal ion cluster, magic number, theoretical modeling of nano particles. Geometric structure, electronic structure, reactivity, magnetic clusters. Bulk to nano transitions, semi-conductivity of nano particles, optical properties, photo fragmentation, coulombic explosion. Carbon nano structures, carbon molecules, Carbon clusters, carbon nano tubes.

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