Islamic University of Science & Technology

Syllabi for PhD Entrance Test

Subject: CHEMISTRY

Part A:	**Research Methodology**	**Marks 35**
Part B:	**Subject Specific**	**Marks 35**

Part A: Research Methodology

Section I

Research Fundamentals, Aims and objectives of research, Types of research: basic, novel and applied research. Tools for searching a Research topic: books, journals, internet, discussions etc. Research hypothesis; Steps in research design. Publication of research, plagiarism, Intellectual property rights. Quality of research work and papers indexing, impact factor, citation index, H Index. Web resources:

Section II

Basic knowledge of computers and software. General awareness of computer Hardware i.e., CPU and other peripheral devices (input / output and auxiliary storage devices), primary and secondary memory. Basic knowledge of software and programming languages. General awareness of popular commercial software packages and scientific application packages like Chemdraw.

Mathematical tools: Rules for differentiation, derivatives of common functions; Applications of differential calculus including maxima & minima finding (Maximally populated rotational levels, most probable velocity). Integration, Basic rules for integration, Integration by substitution, Integration by parts, Applications of integral calculus in Kinetics (zero, first, second order reactions). Differential equations, second order homogeneous DE and its solution by auxiliary equations method.

Section III

General introduction: Instrumental and non-Instrumental methods of analysis in Chemistry. Errors in measurement. Classification of errors, Determinate/Systematic and indeterminate/ Random errors. Accuracy and precision & reproducibility of a measurement. Mean, Median, Average deviation and standard deviation and variance of data. Confidence interval; Correlation coefficient and regression analysis. Comparison of methods: F-test and T-test; rejection of data based on Q-test. Linear Least squares method. Concepts and difference between sensitivity, LOD and LOQ.

Section IV

Instrumentation, Tools & Techniques of research in chemistry.

Spectroscopic methods: IR, UV-Vis, NMR (^{1}H & ^{13}C) NMR, EPR, NQR and Mass.

Electro analytical methods: pH metry, Conductometry, potentiometry, amperometry

Separation techniques: Chromatography (TLC, SEC, HPLC and GC)

Part B: Subject Specific

Section 1

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 and 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. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.

Section 2

Basic principles of quantum mechanics; operator algebra, Postulates. Particle-in-a box, harmonic oscillator, rigid rotator and the hydrogen atom problems, tunneling; shapes of atomic orbitals. Orbital and spin angular momenta. Variational method; perturbation method up to second order in energy; applications. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.

Group theory: symmetry elements; point groups; character tables; selection rules, applications.

Chemical thermodynamics: Laws, and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle. Elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.

Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.

Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye- Huckel theory; electrolytic conductance –Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.

Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.

Solid state: Crystal structures; Bragg's law and applications; band structure of solids.

Section 3

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 non-benzenoid compound– 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 – 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, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.

Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination.

Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry. Synthesis /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.

Section 4

Chromatography, stationery and mobile phase. Column, paper and thin layer chromatography. HPLC: Plate theory, Rate theory, Van-Deemter-Equation, Resolution, Retention time and other basic parameters. Basic difference between HPLC and conventional LC. Packing materials and equipments, Detectors, Advantages and Applications,

GC: Instrumentation: Columns and stationary phases, Detectors:- TCD, FID and Electron Capture Detector, Factors affecting the efficiency of the column, Qualitative and quantitative analysis based on peak height and peak area.

Polymers, Classification: Isotactic, Atactic, Syndiotactic & Graft polymers. Polymerization mechanism: Chain polymerization, Step polymerization. Polydispersion and average molecular weight concept. Number, Weight & viscosity average molecular weights, Measurement of molecular weights: End-group, Membrane osmometry, light scattering and viscometry.

Nanoscience and nanotechnology, Nanostructures in nature, Surface effects of nanomaterials, Surface plasmon resonance, Quantum size effects, Effect of size on properties, reactivity, optical, electrical, and magnetic properties.

Electrogravimetric analysis, coulometry, amperometry, linear sweep and cyclic voltammetry

Thermo gravimetric analysis (TGA), Apparatus, Methodology, Applications of TGA for quantitative analysis (CaC_2O_4. H_2O, $CuSO_4$. $5H_2O$, dolomite ore,) and problems based on TGA.

Differential thermal analysis (DTA): Apparatus, Methodology, Applications. Comparative study of TGA and DTA, Interpretation of TGA and DTA curves of important compounds.