Ph.D. Entrance Syllabus Department of Chemistry & Biochemistry Sharda School of Basic Sciences and Research

Subject: Chemistry

Course	Content
Physical Chemistry	Quantum Mechanics: Basic principles of quantum mechanics: Postulates; operator algebra; exactly-solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunnelling. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance. Chemical thermodynamics: Laws, state and path functions 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 gasses, and solutions. 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. Polymer chemistry: Molar masses; kinetics of polymerization
Organic Chemistry	IUPAC nomenclature of organic molecules including regio- and stereoisomers. Concept of aromaticity: Benzenoid and non-benzenoid compounds. Organic reactive intermediates: Generation, stability, and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, and asymmetric induction. Reaction mechanism, common name reactions, and rearrangement; important reagents (organic, inorganic, organometallic, and

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enzymatic) for functional group transformation. Concepts in organic synthesis: Retrosynthesis, disconnection, and protecting groups. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction, Resolution – optical and kinetic. Pericyclic reactions – electrocyclization, cycloaddition, sigmatropic rearrangements, and other related concerted 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. Structure determination of organic compounds by IR, UV-Vis, ¹H & ¹³C NMR, and Mass spectroscopic techniques.

Inorganic Chemistry

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Chemistry of s, p, d, and f block elements; Structure and bonding in homo- and heteronuclear molecules including shapes of molecules (VSEPR Theory); Periodic properties; Concepts of acids and bases; Non-aqueous solvents; Organometallic compounds: synthesis, bonding and structure, and reactivity; Organometallics in Homogeneous Catalysis; Cages and metal clusters; Bioinorganic chemistry: photosynthesis, porphyrins, metalloenzymes, oxygen transport, electron-transfer reactions; nitrogen fixation, metal complexes in medicine; Characterization of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, MS and microscopic techniques; Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis; Coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.

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