

Khaja Bandanawaz University

Faculty of Science

Department of Chemistry

Chemistry Syllabus for the PhD Entrance Exam, 2025

Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).
3. Concepts of acids and bases, Hard-Soft acid base concept, non-aqueous solvents.
4. Main group elements and their compounds and properties
5. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.
6. Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis.
7. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
8. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.

Physical Chemistry:

1. 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; tunneling.
2. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π -electron systems.
3. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
4. Molecular spectroscopy: IR and Raman activities – selection rules; basic principles of magnetic resonance.
5. 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; LeChatelier principle

6. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
7. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
8. 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.
9. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
10. Polymer chemistry: Molar masses; kinetics of polymerization.

Organic Chemistry

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes.
4. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
5. Common named reactions and rearrangements – applications in organic synthesis.
6. Pericyclic reactions – electrocycloaddition, cycloaddition, sigmatropic rearrangements and other related concerted reactions.
7. Structure determination of organic compounds by IR, UV-Vis, ^1H & ^{13}C NMR and Mass spectroscopic techniques.