Syllabus for Ph.D. Entrance Exam

Chemistry

1. Chemical periodicity: Atomic structure, electronic configuration of atoms and periodic properties of elements.
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR theory and hybridization).
3. Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents.
4. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.
5. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
6. Organometallic compounds: synthesis, bonding, 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.
9. Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.
10. Stoichiometry: Problems based on balanced chemical equations.

11. 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.
12. Approximate methods of quantum mechanics: Variation principle; perturbation theory up to first order in energy; applications.
13. Chemical bonding in diatomics: elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.
14. Chemical applications of group theory: symmetry elements; point groups; character tables; selection rules.
15. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.

16. 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 gases, and solutions.
17. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
18. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
19. 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.
20. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
21. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

22. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
23. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
24. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
25. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
26. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
27. 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.
28. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
29. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst-controlled reactions; determination of enantiomeric and diastereomeric excess; enantio discrimination. Resolution – optical and kinetic.
30. Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
31. Structure determination of organic compounds by IR, UV-Vis, 1H & 13C NMR and Mass spectroscopic techniques.