PhD Syllabus Chemistry

General

Physical chemistry:

1. Basic principles of quantum mechanics: Postulates; operator algebra; exactly solvable systems: particle-in-a-box, including shapes of atomic orbitals; orbital and spin angular momenta.
2. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
3. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.
4. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.
5. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch’s law and its applications; ionic equilibria; conductometric and potentiometric titrations.
6. Solid state: Crystal structures; Bragg’s law and applications; band structure of solids.
7. Polymer chemistry: Molar masses; kinetics of polymerization.
8. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

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. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
7. Structure determination of organic compounds by IR, UV-Vis, 1H & 13C NMR and Mass spectroscopic techniques.

Inorganic chemistry:

2. Chemical periodicity
3. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules - VBT & MOT
5. Chemistry of the main group elements and their compounds. Allotropy, synthesis, bonding and structure.
7. Coordination complexes: Nomenclature, Isomerism, Transition metal carbonyls

**Specialization**

**Physical Chemistry:**

1. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
2. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
3. 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.
5. 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.

**Organic Chemistry:**

2. 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.
5. Chemistry of natural products such as carbohydrates, terpenes etc.

**Inorganic Chemistry:**


3. Radioactivity: Characteristics of radioactive decay, Decay kinetics, types of decay, \(\alpha\), \(\beta\), \(\gamma\)-emissions, artificial radioactivity. Nuclear fission and fusion; Nuclear Reactors: Classification of reactors, reactor power, and application of radioactivity

4. Coordination chemistry: Ligand, Chelate effect, crystal field, Spectrochemical Series, Nephauxatic effect, tetragonal distortion, Color, spectral and magnetic properties, Spinels.