Applied Chemistry

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: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.
- 5. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.
- 6. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
- 7. Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis.
- 8. Cages and metal clusters.
- 9. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
- 10. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.
- 11. Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.
- 12. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

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. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
- 3. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
- 4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π -electron systems.
- 5. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.

- 6. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities selection rules; basic principles of magnetic resonance.
- 7. 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.
- 8. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities calculations for model systems.
- 9. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
- 10. 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.
- 11. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.
- 12. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
- 13. Polymer chemistry: Molar masses; kinetics of polymerization.
- 14. 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.
- 4. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.

- 5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
- 6. Common named reactions and rearrangements applications in organic synthesis.
- 7. 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.
- 8. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
- 9. 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.
- 10. Pericyclic reactions electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
- 11. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).
- 12. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.
- 13. Structure determination of organic compounds by IR, UV-Vis, ¹H & ¹³C NMR and Mass spectroscopic techniques.

Interdisciplinary topics

- 1. Introduction to material science
- 2. Agrochemicals & fertilizers
- 3. Research methodology
- 4. Medicinal chemistry.
- 5. Supramolecular chemistry.
- 6. Environmental chemistry.