PhD Syllabus 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 _-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.
9. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
10. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
11. 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;
12. Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.
13. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
14. 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.
15. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
16. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
17. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
18. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
19. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
20. Synthesis and reactivity of common heterocyclic compounds containing one heteroatom (O,N,S).
21. Structure determination of organic compounds by IR, UV-Vis, 1H & 13C NMR and Mass spectroscopic techniques.

22. Common named reactions and rearrangements – applications in organic synthesis.
23. 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.
24. 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.
25. Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
26. Chemistry of natural products such as carbohydrates, terpenes etc.

27. Atomic Structure : de Broglie matter waves. Heisenberg uncertainty principle. Atomic orbitals. Quantum numbers. Aufbau and Paulis exclusion principles. Hund's multiplicity rule. Hydrogen atom: energy of orbitals, atomic spectra, P-fund, bracket series.
28. Electronic configuration of elements, effective nuclear charge and shielding; radial and angular wave
functions and distribution curves, shape of s,p,d orbitals and their characteristics
29. Chemical periodicity
30. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules - VBT & MOT
31. Concepts of acids and bases.
32. Chemistry of the main group elements and their compounds. Allotropy, synthesis, bonding and structure.
33. Nernst Equation, Electrochemical series, Formal Potential and its application: Effect of pH**,** complexation, solubility; Disproportionation and comproportionation reaction, Principles involved in the extraction of the elements.
34. Coordination complexes: Nomencleture, Isomerism, Transition metal carbonyls
35. Classical and non-classically bonded organometallic compounds, 18 electron rule in Organometallic complexes-Ionic and Covalent Model, Metal-alkyl complexes, structure and bonding of methyl-Lithium complex.
36. Grignard reagents, _ complexes- metal hydrides.
Metalolefin complexes, Ziese's salt, Transition metal carbene complexes, Metallocenes and Metal arenes. Multidecker compounds: Fluxional behavior of organometallic compounds.
37. Elements of life, metallo-biomolecules– enzymes and proteins, their differences; Na^{+} , K^{+} pump, Ca^{2+} transport.Super oxide dismutase, Catalase, Peroxidase, Cytochrome c Oxidase, Cytochrome P – 450.
38. Natural Oxygen carriers : Hemoglobin, Myoglobin, Hemocyanin, Hemerythrin– mechanism and model compounds. Iron – Sulphur proteins, Cytochromes, Nitrogenase- biological nitrogen fixation
39. Radioactivity: Characteristics of radioactive decay, Decay kinetics, types of decay, _, _, _-emissions, artificial radioactivity. Nuclear fission and fusion; Nuclear Reactors: Classification of reactors, reactor power, and application of radioactivity
40. Coordination chemistry: Ligand, Chelate effect, crystal field, Spectrochemical Series, Nephauxatic effect, tetragonal distortion, Color, spectral and magnetic properties, Spinels.