

## Syllabus for Ph. D. Admission 2023

The Ph. D. students will be selected based on written test and interview. The syllabus of the subject is given below.

### Chemistry

#### Section 1: Physical Chemistry

Structure: Postulates of quantum mechanics. Time dependent and time independent Schrödinger equations. Born interpretation. Particle in a box. Harmonic oscillator. Rigid rotor. Hydrogen atom: atomic orbitals. Multi-electron atoms: orbital approximation. Variation and first order perturbation techniques. Chemical bonding: Valence bond theory and LCAO-MO theory. Hybrid orbitals. Applications of LCAO-MO to  $H_2^+$ ,  $H_2$  and other homonuclear diatomic molecules, heteronuclear diatomic molecules like HF, CO, NO, and to simple delocalized–electron systems. Hückel approximation and its application to annular, –electron systems. Symmetry elements and operations. Point groups and character tables. Origin of selection rules for rotational, vibrational, electronic and Raman spectroscopy of diatomic and polyatomic molecules. Einstein coefficients. Relationship of transition moment integral with molar extinction coefficient and oscillator strength. Basic principles of nuclear magnetic resonance: nuclear g factor, chemical shift, nuclear coupling.

Equilibrium: Laws of thermodynamics. Standard states. Thermochemistry. Thermodynamic functions and their relationships: Gibbs-Helmholtz and Maxwell relations, van't Hoff equation. Criteria of spontaneity and equilibrium. Absolute entropy. Partial molar quantities. Thermodynamics of mixing. Chemical potential. Fugacity, activity and activity coefficients. Chemical equilibria. Dependence of equilibrium constant on temperature and pressure. Non-ideal solutions. Ionic mobility and conductivity. Debye-Hückel limiting law. Debye-Hückel-Onsager equation. Standard electrode potentials and electrochemical cells. Potentiometric and conductometric titrations. Phase rule. Clausius- Clapeyron equation. Phase diagram of one-component systems:  $CO_2$ ,  $H_2O$ , S; two component systems: liquid-vapour, liquid-liquid and solid-liquid systems. Fractional distillation. Azeotropes and eutectics. Statistical thermodynamics: microcanonical and canonical ensembles, Boltzmann distribution, partition functions and thermodynamic properties.

Kinetics: Transition state theory: Eyring equation, thermodynamic aspects. Potential energy surfaces and classical trajectories. Elementary, parallel, opposing and consecutive reactions. Steady state approximation. Mechanisms of complex reactions. Unimolecular reactions. Kinetics of polymerization and enzyme catalysis. Fast reaction kinetics: relaxation and flow methods. Kinetics of photochemical and photophysical processes.

Surfaces and Interfaces: Physisorption and chemisorption. Langmuir, Freundlich and BET isotherms. Surface catalysis: Langmuir-Hinshelwood mechanism. Surface tension, viscosity. Self-assembly. Physical chemistry of colloids, micelles and macromolecules.

#### Section 2: Inorganic Chemistry

Main Group Elements: Hydrides, halides, oxides, oxoacids, nitrides, sulfides – shapes and reactivity. Structure and bonding of boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes. Allotropes of carbon. Chemistry of noble gases, pseudohalogens, and interhalogen compounds. Acid-base concepts.

Transition Elements: Coordination chemistry – structure and isomerism, theories of bonding (VBT, CFT, and MOT). Energy level diagrams in various crystal fields, CFSE, applications of CFT, Jahn-Teller distortion. Electronic spectra of transition metal complexes: spectroscopic term symbols, selection rules, Orgel diagrams, charge-transfer spectra. Magnetic properties of transition metal complexes. Reaction mechanisms: kinetic and thermodynamic stability, substitution and redox reactions.

Lanthanides and Actinides: Recovery. Periodic properties, spectra and magnetic properties.

Organometallics: 18-Electron rule; metal-alkyl, metal-carbonyl, metal-olefin and metal- carbene complexes and metallocenes. Fluxionality in organometallic complexes. Types of organometallic

reactions. Homogeneous catalysis - Hydrogenation, hydroformylation, acetic acid synthesis, metathesis and olefin oxidation. Heterogeneous catalysis - Fischer-Tropsch reaction, Ziegler-Natta polymerization.

Radioactivity: Decay processes, half-life of radioactive elements, fission and fusion processes.

Bioinorganic Chemistry: Ion ( $\text{Na}^+$  and  $\text{K}^+$ ) transport, oxygen binding, transport and utilization, electron transfer reactions, nitrogen fixation, metalloenzymes containing magnesium, molybdenum, iron, cobalt, copper and zinc.

Solids: Crystal systems and lattices, Miller planes, crystal packing, crystal defects, Bragg's law, ionic crystals, structures of AX, AX<sub>2</sub>, ABX<sub>3</sub> type compounds, spinels, band theory, metals and semiconductors.

Instrumental Methods of Analysis: UV-visible spectrophotometry, NMR and ESR spectroscopy, mass spectrometry. Chromatography including GC and HPLC. Electroanalytical methods- polarography, cyclic voltammetry, ion-selective electrodes. Thermoanalytical methods.

### **Section 3: Organic Chemistry**

Stereochemistry: Chirality of organic molecules with or without chiral centres and determination of their absolute configurations. Relative stereochemistry in compounds having more than one stereogenic centre. Homotopic, enantiotopic and diastereotopic atoms, groups and faces. Stereoselective and stereospecific synthesis. Conformational analysis of acyclic and cyclic compounds. Geometrical isomerism. Configurational and conformational effects, and neighbouring group participation on reactivity and selectivity/specificity.

Reaction Mechanisms: Basic mechanistic concepts – kinetic *versus* thermodynamic control, Hammond's postulate and Curtin-Hammett principle. Methods of determining reaction mechanisms through identification of products, intermediates and isotopic labeling. Nucleophilic and electrophilic substitution reactions (both aromatic and aliphatic). Addition reactions to carbon-carbon and carbon-heteroatom (N,O) multiple bonds. Elimination reactions. Reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals. Molecular rearrangements involving electron deficient atoms.

Organic Synthesis: Synthesis, reactions, mechanisms and selectivity involving the following classes of compounds – alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines and amides. Uses of Mg, Li, Cu, B, Zn and Si based reagents in organic synthesis. Carbon-carbon bond formation through coupling reactions - Heck, Suzuki, Stille and Sonogoshira. Concepts of multistep synthesis - retrosynthetic analysis, strategic disconnections, synthons and synthetic equivalents. Umpolung reactivity – formyl and acyl anion equivalents. Selectivity in organic synthesis – chemo-, regio- and stereoselectivity. Protection and deprotection of functional groups. Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxiliaries. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Michael addition reaction. Stereoselective addition to C=O groups (Cram and Felkin-Anh models). Pericyclic Reactions and Photochemistry: Electrocyclic, cycloaddition and sigmatropic reactions. Orbital correlations - FMO and PMO treatments. Photochemistry of alkenes, arenes and carbonyl compounds. Photooxidation and photoreduction. Di- $\pi$ -methane rearrangement, Barton reaction.

Heterocyclic Compounds: Structure, preparation, properties and reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline.

Biomolecules: Structure, properties and reactions of mono- and di-saccharides, physicochemical properties of amino acids, chemical synthesis of peptides, structural features of proteins, nucleic acids, steroids, terpenoids, carotenoids, and alkaloids.

Spectroscopy: Applications of UV-visible, IR, NMR and Mass spectrometry in the structural determination of organic molecules.

# Physics

## **Section 1: Mathematical Physics**

Linear vector space: basis, orthogonality and completeness; matrices; vector calculus; linear differential equations; elements of complex analysis: Cauchy- Riemann conditions, Cauchy's theorems, singularities, residue theorem and applications; Laplace transforms, Fourier analysis; elementary ideas about tensors: covariant and contravariant tensor, Levi-Civita and Christoffel symbols.

## **Section 2: Classical Mechanics**

D'Alembert's principle, cyclic coordinates, variational principle, Lagrange's equation of motion, central force and scattering problems, rigid body motion; small oscillations, Hamilton's formalisms; Poisson bracket; special theory of relativity: Lorentz transformations, relativistic kinematics, mass-energy equivalence.

## **Section 3: Electromagnetic Theory**

Solutions of electrostatic and magnetostatic problems including boundary value problems; dielectrics and conductors; Maxwell's equations; scalar and vector potentials; Coulomb and Lorentz gauges; Electromagnetic waves and their reflection, refraction, interference, diffraction and polarization; Poynting vector, Poynting theorem, energy and momentum of electromagnetic waves; radiation from a moving charge.

## **Section 4: Quantum Mechanics**

Postulates of quantum mechanics; uncertainty principle; Schrodinger equation; one-, two- and three-dimensional potential problems; particle in a box, transmission through one dimensional potential barriers, harmonic oscillator, hydrogen atom; linear vectors and operators in Hilbert space; angular momentum and spin; addition of angular momenta; time independent perturbation theory; elementary scattering theory.

## **Section 5: Thermodynamics and Statistical Physics**

Laws of thermodynamics; macro states and microstates; phase space; ensembles; partition function, free energy, calculation of thermodynamic quantities; classical and quantum statistics; degenerate Fermi gas; black body radiation and Planck's distribution law; Bose-Einstein condensation; first and second order phase transitions, phase equilibria, critical point.

## **Section 6: Atomic and Molecular Physics**

Spectra of one- and many-electron atoms; LS and jj coupling; hyperfine structure; Zeeman and Stark effects; electric dipole transitions and selection rules; rotational and vibrational spectra of diatomic molecules; electronic transition in diatomic molecules, Franck-Condon principle; Raman effect; NMR, ESR, X-ray spectra; lasers: Einstein coefficients, population inversion, two and three level systems.

## **Section 7: Solid State Physics and Electronics**

Elements of crystallography; diffraction methods for structure determination; bonding in solids; lattice vibrations and thermal properties of solids; free electron theory; band theory of solids: nearly free electron and tight binding models; metals, semiconductors and insulators; conductivity, mobility and effective mass; optical, dielectric and magnetic properties of solids; elements of superconductivity: Type-I and Type II superconductors, Meissner effect, London equation.

Semiconductor devices: diodes, Bipolar Junction Transistors, Field Effect Transistors; operational amplifiers: negative feedback circuits, active filters and oscillators; regulated power supplies; basic digital logic circuits, sequential circuits, flip-flops, counters, registers, A/D and D/A conversion.

## **Section 8: Nuclear and Particle Physics**

Nuclear radii and charge distributions, nuclear binding energy, Electric and magnetic moments; nuclear models, liquid drop model: semi-empirical mass formula, Fermi gas model of nucleus, nuclear shell model; nuclear force and two nucleon problem; alpha decay, beta-decay, electromagnetic transitions in nuclei; Rutherford scattering, nuclear reactions, conservation laws; fission and fusion; particle accelerators and detectors; elementary particles, photons, baryons, mesons and leptons; quark model.

## Renewable Energy

- Unit I • Types of Non-Conventional energy sources, Overview of nonconventional energy resources,  
• Solar energy: Fundamental and its applications, devices for thermal collection, solar photovoltaics: Fundamental and its applications
- Unit II • Biomass-introduction, and their applications. Conversion of biomass into a suitable form, types of the conversion process. Direct combustion of biomass-present and past usage, Gasifiers, Biofuels, Importance of biofuels, Production of bio-diesel plant from plants, Production of biodiesel from algae, Biogas systems and its applications: Structure of Biogas power plant, classification of biogas digesters,
- Unit III • Wind energy: analysis of wind speeds, different types of wind turbines, factors for site selection, performance characteristics etc. Wind energy farms • Geothermal Energy: Introduction, structure of earth's interior, plate tectonic theory, geothermal sites, geothermal field, geothermal resources, geothermal power generation through flash steam system and binary cycle system, global status of power production from geothermal resources
- Unit IV • Tidal, wave and ocean thermal energy conversion plants • Small hydropower: Introduction, classification of small hydropower stations, classification of water turbines, impulse turbine, • Hybrid energy systems: Introduction, the need for hybrid systems, types of hybrid systems,

## Biology

- Biochemistry: Biomolecules - structure and function; Biological membranes, carbohydrates, lipids, amino acids and nucleic acids; Enzymes - Classification, Enzyme kinetics.
- Microbiology: Bacterial classification and diversity; Microbial Ecology - microbes in marine, freshwater and terrestrial ecosystems.
- Immunology: Innate and adaptive immunity, humoral and cell mediated immunity; Antibody structure and function; Molecular basis of antibody diversity; T cell and B cell development;
- Recombinant DNA technology: Restriction and modification enzymes; Vectors - plasmids, bacteriophage and other viral vectors, cosmids, Ti plasmid, bacterial and yeast artificial chromosomes;
- Molecular tools: Polymerase chain reaction; DNA/RNA labelling and sequencing; Southern and northern
- Genetics: Mendelian inheritance; Gene interaction.
- Microbial genetics - transformation, transduction and conjugation; Horizontal gene transfer and transposable elements.
- Cell Biology: Prokaryotic and eukaryotic cell structure; Cell cycle and cell growth control; Cell-cell communication; Cell signaling and signal transduction; Post-translational modifications; Protein trafficking; Cell death and autophagy; Extracellular matrix.
- Molecular Biology: Molecular structure of genes and chromosomes; Mutations and mutagenesis; Regulation of gene expression; Nucleic acid - replication, transcription, splicing, translation and their regulatory mechanisms; Non-coding and micro RNA; RNA interference; DNA damage and repair.
- Bioenergy and Biofuels: Introduction to Bioresources, Green Technology: utilization of bioresources from animals, plants, and microbes for use of cosmetic products. Utilization of plant and animal wastes for production of eco-friendly biofuels (biodiesel and bioethanol) and the possibility of using microbes to produce bio-hydrogen as a source of future fuel. Biofertilizers, Biopesticides & Organic Farming.

## **Humanities and Social Sciences**

Multi-genre literatures in English, Comparative context, anglophone and literatures from India in English translation, Literary criticism and theory, History of English literature

Sociological Theory, Research Methodology and Methods, Sociological Concepts, Agrarian Sociology and Rural Transformation, Family, Marriage and Kinship, Indian Society / Sociology of India, Social Movements, Sociology of Development