Entrance Exam for Ph.D Syallabus (Chemistry)

INORGANIC CHEMISTRY

1. Sructure and Bonding : Atomic orbitals, electronic configura-tion of atoms (L-S coupling) and the periodic properties of ele-ments; ionic radili, ionisation potential, electron affinity, elec-tronegativity; concept of hybridization. Molecular orbitals and electronic configuration of homonuclear and heteronuclear di-atomic molecules. Shapes of polyatomic molecules; VSEPR, theory Symmetry elements and point groups for simple molecules.Bond lengths, bond angles, bond order and bond en-ergies. Types of Chemical Bond (weak and strong) intermolecu-lar forces, structure of simple ionic and covalent solids, lattice energy.

2. Acids and bases : Bronsted and Lewis acids and bases, pH and pKa, acid-based concept in non-aqueous media; HSAB concept. Buffer solution.

3. Redox Reactions : Oxidation numbers. Redox potential. Elec- trochemical series. Redox indicators.

4. Energetics and Dynamics of Chemical Reactions: Law of conservation of energy.Energy and enthalpy of reactions. Entropy, free-energy, relation-ship between free energy change and equilibrium. Rates of chemical reactions (first-and second-order reaction). Arrhenius equation and concept of transition state. Mechanisms, includ-ing SN1 and SN2 reactions, electron transfer reactions, cataly-sis. Colligative properties of solutions.

5. Aspects of s.p.d.f. Block Elements

6. **IUPAC Nomenclature of simple Inorganic Compounds**

7. Chemistry of Non-transition Elements

8. Chemistry of Transition Elements

9. Chemistry of Lanthanides and Actinides: Spectral and magnetic properties; Use of lanthanide compounds as shift reagents.

10. Organometallic chemistry of Transition Elements: Synthesis,structure and bonding, organometallic reagents in organic synthesis and in homogeneous catalytic reactions (hydrogenation,hydrodormaylation, isomerisation and polymerisation); Pi-acid
metal complexes, activation of small molecules by coordination.

11. Bionorganic Chemistry

12. Data Analysis: Types of errors, propagation of errors, accuracy and precision, leastsquares analysis, average standard deviation.

PHYSICAL CHEMISTRY

1. Quantum Chemistry: Planck's quantum theory, wave-particle duality. Uncertainity Principle. operators and commutation re-lations : postulates of quantum mechanics and Schrodinger equation free particle. particle in a box, degeneracy, harmonic oscil-lator, rigid rotator and the hydrogen atom. Angular momentum, including spin; coupling of angular momenta including spin-orbit coupling.

2. Born-Oppenheimer approximation. Hydrogen molecule ion. LCAO-MO and AB treatments of the hydrogen molecule; elec-tron density. forces and their role in chemical binding.Hybridisation and valence

3. Spectroscopy : Theoretical treatment of rotational, vibrational and electronic spectroscopy. Principles of magnetic resonance, Mossbauer and photoelectron spectroscopy.

4. Thermodynamics : First law of thermodynamics, relation between Cp and Cv; enthalpies of physical and chemical changes;temperature dependence of enthalpies. second law of thermo-dynamics, entropy. Gibbs-Helmoholtz equation. Third law ofthermodynamics and calculation of entropy.

5. Chemical Equilibrium : Free energy and entropy of mixing, pertial moler quantities, Gibbs-Duhem equation. Equilibrium constant. temperature-dependence of equilibrium constant, phase diagram of one and two-component systems, phase rule.

6. Ideal and Non-ideal solutions. excess functions, activities, concept of hydration number : activities in electrolytic solutions; mean ionic activity coefficient; Debye-Huckel treatment of dilute electrolyte solutions.

7. Electrochemistry : Electrochemical cell reactions, Nernst equation, Electrode Kinetics, electical double layer, electode/electrolyte interface, Batteries, primary & secondary Fuel cells, corrosion and corrosion prevention.

8. Surface Phenomena : Surface tension,adscription on solids, electrical phenomena at interphaces, including electrokinetic, micelles and reverse micelles : solubilization, micro-emulsions.Application of photelectron spectroscopy. ESCA and Auger spectroscopy to the study of surfaces.

9. Reaction Kinetics : Methods of determining rate laws. Mechanisms of photochemical, chain and oscillatory reactions. Collision theory of reaction rates; steric factor, treatment of unimolecular reactions. Theory of absolute reaction rates omparision of results with Eyring and Arrhenius equations. Ionicreaction : salt effect. Homogeneous catalysis and Michaelis-Menten kinetics; heterogeneous catalysis.

10. Fast Reaction : Luminescence and Energy transfer processes.Study of kinetics by stoppedflow technique, realization method,flash photolysis and magnetic resonance method.

11. Macromolecules : Number-average and weight average molecular weights; determination of molecular weights. Kinetics of polymerisation. Stereochemistry and mechanism of polymerisation.

12. Solids : Dislocation in solids, schottky and Frenkel defects, Electrical properties; Insulators and semiconductors; superconductors; band theory of solids, Solid-state reactions.

13. Nuclear Chemistry : Radioactive decay and equilibrium. Nuclearreactions; Q value, cross sections, types of reactions, Chemicaleffects of nuclear transformations; fission and fusion, fission products and fission yields. Radioactive techniques; tracer technique, neutron activation analysis, counting techniques such asG.M. ionization and proportional counter.

14. Topics in Analytical Chemistry : Adsorption partition, exclusion electrochromatography. Solvent extraction and ion exchangemethods. Application of atomic and molecular absorption andemission spectroscopy in quantitative analysis Light scattering techniques including nephelometry and Raman spectroscopy. Electronalytical techniques : voltammetry, cyclic, voltammetry, polarography, amperometry, colometry and conductometry ion-
elective electrodes, annodic stripping voltammetry : TGA, DTA,DSC and online analysers.

ORGANIC CHEMISTRY

1 IUPAC Nomenclature of simple Organiccompounds,Aromaticity : Huckel's rule and concept of aromaticty (n) annulenes and heteroannulenes, fullerenes (C60)

2. Stereochemistry and conformational Analysis : Nwere method of asymmetric synthesis (including enzymatic and catalyticnexus), enantio and diastereo selective synthesis. Effects of con-formation on reactivity in acyclic compounds and cyclohexanes.

3. Selective Organic Name Reactions

4. Mechanisms of Organic Reaction : Labelling and Kinetio isotope effects, Hamett equation, (sigma-rho) relationship, non-classical carbonium ions, neighbouring group participation.

5. Pericyclic Reactions : Selection rules and stereochemistry of electrocyclic reactions, cycloaddition and sigmatropic shifts, Sommelet, Hauser, Cope and Claisen rearrangements.

6. Heterocyclic Chemistry : Synthesis and reactivity of furan thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, fischer indole synthesis.

7. Reagents in Organic Synthesis : Use of the following reagents in organic synthesis and functional group transformations; Com- plex metal hybrides, Gilmen's reagent, lithium dimethylcuprate, lithium disopropylamide (LDS\A) dicyclohexyicarbodimide, 1,3-dithiane (reactivity umpolung), trimethylisilyl iodide, tri-nbutyltin hybride, Woodward and prevost hydroxylation, osmiumtetroxide, DDZ, selenium dioxide, phase transfer catalysis, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinsonscatalyst, Baker yeast.

8. Chemistry of Natural products : Famillarity with methods of structure elucidation and biosynthesis of alkaloids, terponoids, steroids, carbohydrates and protains.

9. Bioorganic Chemistry : Elementary structure and function of biopolymers such as proteins and nucleic acids.

10. Photochemistry : Cis-trans isomeriation, Paterno-Buchi reaction, Norrish Type I and II reactions, photoreduction of ketones, dipinethane rearrangement, photochemistry of areanes.

11. Spectroscopy : Applications of mass, UV-VIS, IR and NMR spectroscopy for structural elucidation of compound.