UPSC Mains Chemistry Optional Paper-I Syllabus

1. Atomic Structure:

Heisenberg's uncertainty principle Schrodinger wave equation (time independent); Interpretation of wave function, particle in one-dimensional box, quantum numbers, hydrogen atom wave functions; Shapes of s, p and d orbitals.

2. Chemical bonding:

Ionic bond, characteristics of ionic compounds, lattice energy, Born-Haber cycle; covalent bond and its general characteristics, polarities of bonds in molecules and their dipole moments; Valence bond theory, concept of resonance and resonance energy; Molecular orbital theory (LCAO method); bonding H_2 +, H_2 He_2 + to Ne₂, NO, CO, HF, CN⁻, Comparison of valence bond and molecular orbital theories, bond order, bond strength and bond length.

3. Solid State:

Crystal systems; Designation of crystal faces, lattice structures and unit cell; Bragg's law; X-ray diffraction by crystals; Close packing, radius ratio rules, calculation of some limiting radius ratio values; Structures of NaCl, ZnS, CsCl, CaF₂; Stoichiometric and nonstoichiometric defects, impurity defects, semi-conductors.



4. The Gaseous State and Transport Phenomenon:

Equation of state for real gases, intermolecular interactions, and critical phenomena and liquefaction of gases; Maxwell's distribution of speeds, intermolecular collisions, collisions on the wall and effusion; Thermal conductivity and viscosity of ideal gases.

5. Liquid State:

Kelvin equation; Surface tension and surface enercy, wetting and contact angle, interfacial tension and capillary action.

6. Thermodynamics:

Work, heat and internal energy; first law of thermodynamics.

Second law of thermodynamics; entropy as a state function, entropy changes in various processes, entropy-reversibility and irreversibility, Free energy functions; Thermodynamic equation of state; Maxwell relations; Temperature, volume and pressure dependence of U, H, A, G Cp and Cv, & and ß; J-T effect and inversion temperature; criteria for equilibrium, relation between equilibrium constant and thermodynamic quantities; Nernst heat theorem, introductory idea of third law of thermodynamics.

7. Phase Equilibria and Solutions:

Clausius-Clapeyron equation; phase diagram for a pure substance; phase equilibria in binary systems, partially miscible liquids--upper and lower critical solution temperatures; partial molar quantities, their significance and determination; excess thermodynamic functions and their determination.

8. Electrochemistry:

Debye-Huckel theory of strong electrolytes and Debye-Huckel limiting Law for various equilibrium and transport properties.

Galvanic cells, concentration cells; electrochemical series, measurement of e.m.f. of cells and its applications fuel cells and batteries.

Processes at electrodes; double layer at the interface; rate of charge transfer, current density; overpotential; electroanalytical techniques: amperometry, ion selective electrodes and their use.

9. Chemical Kinetics:

Differential and integral rate equations for zeroth, first, second and fractional order reactions; Rate equations involving reverse, parallel, consecutive and chain reactions; Branching chain and explosions; effect of temperature and pressure on rate constant. Study of fast reactions by stop-flow and relaxation methods. Collisions and transition state theories.

10. Photochemistry:

Absorption of light; decay of excited state by different routes; photochemical reactions between hydrogen and halogens and their quantum yields.

11. Surface Phenomena and Catalysis:

Adsorption from gases and solutions on solid adsorbents; Langmuir and B.E.T. adsorption isotherms; determination of surface area, characteristics and mechanism of reaction on heterogeneous catalysts.

12. Bio-inorganic Chemistry:

Metal ions in biological systems and their role in ion-transport across the membranes (molecular mechanism), oxygen-uptake proteins, cytochromes and ferrodoxins.

13. Coordination Chemistry:

(i) Bonding in transition of metal complexes. Valence bond theory, crystal field theory and its modifications; applications of theories in the explanation of magnetism and electronic spectra of metal complexes.

(ii) Isomerism in coordination compounds; IUPAC nomenclature of coordination compounds; stereochemistry of complexes with 4 and 6 coordination numbers; chelate effect and polynuclear complexes; trans effect and its theories; kinetics of substitution reactions in square-planar complexes; thermodynamic and kinetic stability of complexes.

(iii) EAN rule, Synthesis structure and reactivity of metal carbonyls; carboxylate anions, carbonyl hydrides and metal nitrosyl compounds.

(iv) Complexes with aromatic systems, synthesis, structure and bonding in metal olefin complexes, alkyne complexes and cyclopentadienyl complexes; coordinative unsaturation, oxidative addition reactions, insertion reactions, fluxional molecules and their characterization; Compounds with metal-metal bonds and metal atom clusters.

14. Main Group Chemistry:

Boranes, borazines, phosphazenes and cyclic phosphazene, silicates and silicones, Interhalogen compounds; Sulphur-nitrogen compounds, noble gas compounds.



15. General Chemistry of 'f' Block Element:

Lanthanides and actinides: separation, oxidation states, magnetic and spectral properties; lanthanide contraction.