Chemistry-I

(Concepts in chemistry for engineering)

Unit I

Atomic and molecular structure

Schrodinger equation. Particle in a box solution and their applications for conjugated molecules and nanoparticles. Molecular orbitals and energy level diagrams of diatomic molecules. Equations for atomic and molecular orbitals. Pi-molecular orbitals of butadiene and benzene and aromaticity. coordination numbers and geometries, Crystal field theory and the energy level diagrams for transition metal ions (octahedral and tetrahedral environment) and their magnetic properties. Band structure of solids and the role of doping on band structures.

Unit II

Spectroscopic techniques and applications

Electronic spectroscopy: Principle and instrumentation, electronic transitions, Chromophores and auxochromes, factors affecting the value of max and intensity of spectral lines. Fluorescence and its applications in medicine. Vibrational and rotational spectroscopy of diatomic molecules: selection rules, expression for energies. Nuclear magnet5ic resonance (1H NMR): Principle, instrumentation, chemical shift, coupling (spin-spin coupling), splitting of peaks, interpretation of 1H NMR of simple molecules; Applications of spectroscopy

Unit III

Intermolecular forces and potential energy surfaces

Ionic, dipolar and van Der Waals interactions. Deviations of real gases from ideal behavior, equations of state of real gases (van der Waals equation of state), and critical phenomena (critical constants and their relation with van der Waals constant). Potential energy surfaces of H3, H2F and HCN and trajectories on these surfaces.

Unit IV

Use of free energy in chemical equilibria

Thermodynamic functions: energy, entropy and free energy. Estimations of entropy and free energies. Free energy and emf. Cell potentials, the Nernst equation and applications. Acid base, oxidation reduction and solubility equilibria. Water chemistry: Hardness of water, units of hardness, problems associated with hardwater, softening of hardwater (lime soda process and zeolite process); Corrosion: Introduction, electrochemical & dry corrosion (mechanism & their comparison), rusting of iron, factors affecting the rate of corrosion, protective measures.

Unit V

Periodic properties

Effective nuclear charge, penetration of orbitals, variations of s, p, d and f orbital energies of atoms in the periodic table, electronic configurations, atomic and ionic sizes, ionization energies, electron affinity and electronegativity, polarizability, oxidation states, hard soft acids and bases, molecular geometries.

Unit VI

Stereochemistry

Representations of 3 dimensional structures, structural isomers and stereoisomers, configurations and symmetry and chirality, enantiomers, diastereomers, optical activity, absolute configurations, determination of R/S configuration, conformational analysis (ethane, propane & butane molecules).

Unit VII

Organic reactions and synthesis of a drug molecule

Introduction; Substitution reactions: Electrophilic, Nucleophilic (SN1 & SN2) and free radical substitution reactions, Friedel Craft alkylation reaction, Halogenation of alkanes; addition reactions: Electrophilic, Nucleophilic and free radical addition reactions, Markovnikov's addition, Anti-markovnikov's addition; elimination (E1 & E2); Synthesis of a commonly used drug molecule.