CHEMISTRY

Unit -1

Analytical Chemistry: Classification of analytical Methods – classical and instrumental. Errors and Evaluation: Definition of terms in mean and median – Types of errors, propagation of errors, accuracy and precision, least squares analysis, average standard deviation.

Analytical Techniques: Principle and applications of adsorption, partition, ion exchange and solvent extraction chromatographic methods – TLC HPLC and GC. Applications of atomic, molecular and emission spectroscopy in quantitative analysis Electroanalytical techniques – cyclic and stripping voltametry, polarography, TGA, DTA, and DSC. Light scattering techniques including nepelometry and Raman spectroscopy.

Unit-2

Structure and Bonding: Atomic orbitals – Types of chemical Bonds (weak and strong) intermolecular forces - Theories of bonding (VB and MO) - Concept of hybridization – shapes of polyatomic molecules – VSEPR theory – Structure of simple ionic and covalent compounds – lattice energy – crystal defects – Insulators and semiconductors, superconductors, Band theory of solids –Solid state reactions.

Acids and Bases : Bronsted and Lewis acids and bases, pH and pKa, acid-base concept in nonaqueous media, HSAB concept, Buffer solution.

Redox Reactions: Oxidation numbers, Redox potential, electrochemical series, Redox indicators, Chemical principles involved in extractions and purification of Iron, Copper, Lead, Zinc and Aluminium.

Unit-3

Nuclear Chemistry: Radioactive decay and equilibrium, Nuclear reactions: Q valve, cross sections, types of reactions, Nuclear transmutations, fission and fusion Radioactive techniques-tracer technique, neutron activation analysis. G.M, Ionization and proportional counters. Radiolysis of water – G value, dosimeters and Hydrated electron.

Chemistry of Non-transition elements: General properties and structure of their halides and oxides. Polymorphism of carbon, phosphorus and sulphur. Synthesis, properties and structure of boranes, carboranes and metallo carboranes - Wade's rule - preparation, properties and structure of borazines & phosphazenes.

Sulphur-nitrogen compounds-Oxides and oxyacids of nitrogen, phosphorous, sulphur and halogens. Interhalogen and noble gas compounds. Isopoly and heteropoly acids and salts.

Unit-4

Chemistry of Transition elements: Co-ordination Chemistry of transition metal ions-Werner's theory – nomenclature and stereo chemistry of co-ordination compounds – stability constants and their determinations – CFT, splitting of d orbitals, CFSE, Jahn Teller effect, charge transfer spectra- spectrochemical series- Term states for d^n ions, Orgel and Tanable- sugano diagram, calculation of D_q B and β parameters.

Inorganic reaction mechanism: Inert and labile complexes-substitution reactions – trans effect – redox and electron transfer reactions. Photochemistry of chromium, ruthenium and cobalt complexes, Chemistry of lanthanides and actinides. Metal carbonyls and metal clusters, Organometallic reagents in organic synthesis- Cayatylic reactions- (hydrogeneation, hydroformylation, isomerization and polymerization) pi-acid metal complexes.

Bioinorganic Chemistry: Metal ions in Biology, Photosynthesis, PSL, PSH, Nitrogen fixation, Oxygen transport and storage, Hemeproteins haemoglobin, cytochrome and ferrodoxins.

Spectroscopy : Applications of nmr,nqr and esr to inorganic compounds.

Unit-5

Chirality. Differentiation of assymmetric and dyssymmetric molecules. Identification of prochiral carbons enantio and diastereoptropic hydrogens in a molecule. Stereochemistry of disubstituted four, five, and six membered saturated alicyclic molecules. Conformational analysis of mono and disubstituted cyclohexanes and piperidines. E-Z nomenclature for isomeric olefins. Stereochemistry of aliphatic nucleophilic substitutions in acyclic and bicyclic systems. Stereochemistry (specific or selective) of dihydroxylations, halogen addition, hydroborations and Diels Alder reaction of suitably substituted olefinic double bonds. Sterospecific E-2 eliminations in erythro–threo isomers. Reduction of ring substituted cyclohexanones to cyclohexanols.

Unit-6

Mechanism of SN-1, reactions in substrates with various types of NGP. Methods of generation and mechanisms of reactions proceeding via carbenes and nitrenes. Concreted reactions: Mechanism of electrocyclic and chelotropic reactions and sigmatropic rearrangements. Photochemical reactions: Mechanisms of Norrish – I and II types, Paterno Buchi and Barton reactions, di-β-methane rearrangements. Rearrangments: Mechanisms of rearrangements proceedings via carbonium ions (Wagner Meerwin pinacol – pinacolone and Demjanov type) and electrophilic heteroatoms (Baeyer Villiger and Curtius type).
Mechanism of nucleophilic substitution in activated aryl halides. Regiochemistry of aryne generation and subsequent additions of o, m and p-substituted aryl halides.

Unit-7

Organic synthesis: Synthesis and any di and trisubstituted benzene derivatives from any mono substituted benzene or benzene itself. Synthesis of simple compounds using C-C bond forming reactions involving Wittig, Wittig Honner, Gilmann Reagents, organolithiums, Grignards, Robinson annulation, Dickmann condensation, Knovenagel, Mannisch, Stork enamine, and Vilsmeyer reactions and Umplolung. (1,3-dithane). Synthetic transformations involving Swern oxidation, Birch Wolf Kishner and metal hydride reductions, catalytic hydrogenations and reagents like tributyltin hydride, trimethylsilyl iodide, LDA, n-BuLi, Raney nickel, NBS Chromium reagents, DCC and Pd. Application of protective group concept (aldelydes, ketones and carboxylic acids) during multistep synthesis. Spectral identification of organic intermediates by IR (functional group) PMR and CMR and mass spectra. (simple molecules only).

Unit-8

Numbering and synthesis of unsubstituded (parent) and alkyl, aryl or acyl (wherever methods are available) substituted furans, pyrroles, thiophene, quionline, iso quinoline and indoles. Reactivity of these compounds towards electrophiles or necleophiles. A study of other non benzenoid aromatics (ferrocences, azulenes, annulenes and fulvenes).

Unit 9

Quantum Chemistry: Plancks' quantum theory, Compton effect, wave particle duality, uncertainty principle, operators: linear and Hermitian, Schrodinger wave equation, postulates of quantum mechanics. Application of Schrodinger equation to particle in a box, harmonic oscillator, rigid rotator and hydrogen atom. Angular momentum: commutation relation, spin orbit interaction Approximation methods: variation theorem, application of variation method to harmonic oscillator, hydrogen and helium atoms. Perturbation theory – application to helium atom. Born – Oppenheimer approximations: LCAO – MO and VB treatments of H_2 molecule. Huckel theory: application to ethylene, butadiene and benzene. Calculation of electron density and bond order. Semi empirical methods: Slater orbital and HF-SCF methods.

Macromolecules: Techniques, mechanism and kinetics of polymerisation, Kinetics of copolymerisation-Molecular weights and their determination. Properties of polymers: glass transition temp. crystallinity of polymers- polymer processing techniques.

Unit-10

Chemical Kinetics: Theories of reaction rate, collision theory, ARRT, comparison- potential energy surfaces- treatment of unimolecular reaction.

Complex reactions: simultaneous, parallel and consecutive reactions. Chain reactions: $H_2.Cl_2$ H_2–Br_2 branching reaction- explosion limit.

Reactions in solution: factors determining reaction rate in solution, dielectric constant and ionic strength, Kinetic isotopic effect, Linear free energy relations. Hammett and Taft equations.

Homogenous Catalysis: acid base catalysis, enzyme catalysis Heterogeneous catalysis: Adsorption, Langmuir and BET adsorption isotherms – mechanism of heterogeneous catalysis.

Thermodynamics: First and second Laws of thermodynamics- relation between c_p and c_v in terms of coefficients of expansion and compressibility. Maxwell relations- partial molar properties- Glibbs' Duhem equation- variation of chemical potential with temperature and pressure-fugacity- Third law and calculation of entropy.

Statistical thermodynamics: Maxwell Boltzmann, Bose-Einstein and Fermi-Dirac distribution-Partition function, translational, rotational and vibrational partition function, calculation of thermodynamic functions, equilibrium constant and heat capacity from partition functions. Einstein and Debye theories of heat capacity of solids., concept of negative absolute temperature.

Nonequilibrium, thermodynamics: Phenomenological laws- Onsagers' reciprocity relation-application to Diffusion potential, electrokinetic phenomena- entropy production.

Unit 11

Group theory: Symmetry elements and symmetry operations, point groups, reducible and irreducible representations – Direct product representation. Orthogonality theorem and its consequences- construction of Character Tale (C_{2v} C_{3v} and C_{2h}) Applications: Selection rules for IR, Raman and electronic spectra, Determining Symmetries of normal vibrational modes of non linear molecules, construction of hybrid orbitals, application to electronic spectra of ethylene and formaldehyde.

Spectroscopy: Rotational Spectra of rigid and non-rigid diatomic rotors, simple polyatomic molecules.

Vibrational Spectra: harmonic and anharmonic oscillator, overtones, Fermi resonane-Raman Spectra. Vibration-rotation Spectra-PQR branches, parallel and perpendicular vibrations.

Electronic Spectroscopy: Spectra of diatomic molecules- Frank condon principle-Morse function. Polyatomic molecules, types of transition, solvent effects.

Spin resonance Spectroscopy: NMR: Origin of nmr signal, Chemical Shift, factors affecting chemical shift and spin spin coupling. NMR Spectra of simple AX and ABX type molecules. ^{13}C and ^{19}F nmr.

ESR: Origin, g-factor, hyperfine structure- Mc Connel equations, Theory and simple applications of Mossbauer and Photoelectron Spectroscopy.

Unit-12

Electrochemistry: Ion-solvent interaction- Born treatment- solvation number and its determination. Ion-ion interaction: activity co-efficient, Debye-Huckel equation for activity coeff - limitations and extension to concentrated solutions. Ion transport: Debye Huckel Orsager equation for conductance- experimental validity. Ion association: its effect on conductance and activity coefficient.

Electrode-electrolyte interface: Structure of double layer- electrode kinetics- overvoltage. Butler – Volmer equation for one electron transfer. Corrosion and Stability of metals: construction and use of Pourbaix and Evans' diagram-Prevention of corrosion, Primary and Secondary cells- Various fuel cells.

Photochemistry: Photophysical processes- Theory of radiationless transition-fluorscence, phosphorescence, fluorescence quenching- Stern-Volmer equation, excimer, exciplexes, Quantum yield measurement, Kinetics of Photochemical reac.