

SYLLABUS FOR THE POST OF LECTURER (10+2) CHEMISTRY:

Quantum Chemistry

Eigen functions and eigen values; Angular momentum and eigen values of angular momentum, spin, Pauli exclusion principle, Schrödinger's equation (time dependent); and wave mechanics of simple systems, particle in one dimensional box, simple harmonic oscillator and the Hydrogen atom. Postulates of quantum, mechanics, Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π -electron systems

Molecular spectroscopy

Spectroscopy: Electromagnetic spectrum, Statement of Born-Oppenheimer approximation.

Rotational spectrum: Moment of inertia, classification of molecules on the basis of moment of inertia. Energy of a rigid diatomic rotor, selection rules for rotational transition and associated spectrum, relative population of rotational levels and spectral intensity, determination of bond length.

Vibrational Spectrum: Classical and quantum mechanical (qualitative) treatment of simple harmonic oscillator, selection rules for vibrational transition, pure vibrational spectrum of a diatomic molecule, determination of force constant, relation of force constant with bond length and bond energy, vibrational degrees of freedom, idea of vibrational frequencies of different functional groups and selection rules.

Ultraviolet Spectroscopy: The electromagnetic spectrum. Beer-Lambert law, molar absorptivity, presentation and analysis of electronic spectra. Types of electronic excitations.

Electrochemistry:

Molar and equivalent conductivity; Migration of ions and Kohlrausch law, Debye-Huckel-Onsager's equation for strong electrolytes. Transport number, Application of conductivity measurements: determination of degree of dissociation and dissociation constants of acids; determination of solubility product of a sparingly soluble salt, Debye-Huckel theory.

Types of reversible electrodes: gas-metal-ion, metal-metal ion, Electrode potential, standard electrode potential, standard hydrogen electrode, reference electrodes, sign conventions. Electrode reactions, Nernst equation, determination of cell E.M.F, electrochemical series and its significance.

Electrolytic and Galvanic cells reversible and irreversible cells, conventional representation of an electrochemical cell. Measurement of EMF of a cell. Calculation of thermodynamic functions of cell reactions (ΔG , ΔH and K). Concentration cells, valency of ions, solubility product and activity coefficient. Corrosion, Batteries. Potentiometric titrations.

Chemical Kinetics & Photochemistry

Rate law, Order of reaction (Zero & First order), Temperature dependence of reaction rates:- Arrhenius equation, concept of activation energy. Theories of chemical kinetics: Simple collision theory based on hard sphere model, evaluation of rate constants of atomic reactions, extension to molecular reactions, limitations. transition state theory. Kinetics salt effects.

Catalysis: Characteristics of catalyzed reactions, Acid-Base catalysis with examples; homogeneous catalysis; enzyme kinetics; Michaelis-Menten equation,

Kinetics of photochemical reactions: Photochemical decomposition of hydrogen iodide. Hydrogen-chlorine and hydrogen-bromine reactions, Comparison with thermal decomposition reactions.

Photochemistry: Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry. Stark-Einstein law, Jablonski diagram qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing), quantum yield, photosensitized reactions, energy transfer processes (simple examples).

States of Matter

Gaseous State: Deviation of gases from ideal behavior, PV isotherms of real gases, continuity of states, the isotherms of vander Waal's equation, relationship between critical constants and vander Waal's constants, the law of corresponding states, reduced equation of state. Root mean square, average and most probable velocities. Maxwell's distribution of molecular velocities, collision number, mean free path and collision diameter,

Liquid State: Liquefaction of gases (based on Joule-Thomson effect) and adiabatic expansion. Intermolecular forces,

Solid State: Symmetry elements in crystals, Lattice planes and Miller indices. X-ray diffraction by crystals, derivation of Bragg's equation and its application.

Laws of Thermodynamics and Chemical Equilibria

First Law of thermodynamics: Heat capacity, heat capacities at constant volume and constant pressure and their relationship. Joule-thomson coefficient and inversion temperature. Calculation of w , q , dU & dH for the expansion of ideal and nonideal (van der Waals) gases under isothermal and adiabatic conditions for reversible. Bond dissociation energy and its calculation from thermo-chemical data. Kirchhoff's equation.

Second law of thermodynamics: Concept of entropy, entropy as a state function, entropy as a function of V & T and P & T , entropy change in physical processes. Entropy as a criteria of spontaneity and equilibrium. Gibbs function (G) and Helmholtz function (A) as criteria for thermodynamic equilibrium and spontaneity. Variation of G and A with P , V and T .

Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.

Equilibrium constant and free energy change. Reaction isotherm and reaction isochore, Clapeyron equation and Clausius-Clapeyron equation, applications. Thermodynamics of elevation in boiling point and depression in freezing point. Activity and activity coefficient. Thermodynamic mixing functions of ideal and nonideal solutions, , Gibbs-Duhem equation, Fugacity of gases, calculation of fugacity from P , T data, concept of ideal and nonideal solutions, Raoult's Law, Henry Law, colligative properties, abnormal molecular mass, Concept of activity and activity co-efficient.

INORGANIC CHEMISTRY:

Chemical Bonding and Periodic Properties:

Chemical Bonding: Ionic Solids: Ionic Structures; Radius ratio effect, Coordination number and limitations of radius ratio rule. Lattice defects; Lattice energy and Born Haber Cycle. Solvation energy and solubility of ionic solids. Polarizing power and polarizability of ions; Fajan's rules. Metallic bond: Characteristics; comparison with ionic and covalent bonds and theories. Valence bond theory: Directional Characteristics of Covalent bond; types of Hybridization. Limitations of VB theory. VSEPR theory: Assumptions; prediction of shapes of molecules. Molecular Orbital Theory: LCAO, Energy level diagram of homo- & heteronuclear diatomic molecules like N_2 , O_2 , F_2 , CO , NO and HCl . Multicentre bonding in electron deficient molecules; Bond strength and Bond energy. Percent ionic character from dipole moment and electronegativity difference. Weak interactions: Hydrogen bonding (concept, types; effect on properties) and Vander Waal forces. Periodic properties: Atomic, Ionic, Metallic and Vander Waal radii. Ionization Potentials, successive ionization potentials; Electronegativity and Electron affinity: Trends in Periodic table and Applications in predicting and explaining the Chemical behavior.

Main group elements and their compounds:

Fluorides and Oxides of Xenon, properties, structure and bonding (VB and MO treatment). Boron Hydrides: Introduction, Nomenclature, Structure and bonding in diborane (including higher boranes), empirical rules for bonding and structure in boranes, Oxides and Oxyacids of

nitrogen (Structure-bonding and Uses). Oxygen fluorides, Oxides and Oxyacids of Sulphur (Properties, Structure-bonding). Halogens: Interhalogens; Polyhalides, Pseudohalogens, (Structure - bonding).

Transition and Inner Transition Elements

Transition Elements: Definition, Classification, Electronic Configuration. Physico-chemical properties: Atomic radii, Ionic radii, Metallic character and related properties; Ionization energies: Variable oxidation states: Ionic, covalent character and Acidic/basic character of compounds of a given transition metal in various oxidation states and stabilization of unusual oxidation states. Spectral and Magnetic properties; calculation and uses of magnetic moment value.

Inner Transition Elements: Comparative account of transition and inner transition elements, d and f orbitals. Lanthanoids: Electronic configuration, Oxidation states, Magnetic properties and Complexing behaviour. Cause and Consequences of lanthanide contraction.

Coordination Compounds:

Werner's Coordination Theory. Effective atomic number: Concept and its significance. IUPAC Nomenclature and Stereochemistry of Coordination numbers (2-6) Isomerism in Coordination Compounds: (including geometrical and optical) Valence bond and Crystal field theories to explain, structure, bonding, magnetic and spectral properties in transition metal complexes (tetrahedral; square planar and octahedral), $10 Dq$; Factors affecting the magnitude of $10 Dq$; pairing energy and CFSE in weak and strong field ligands. Spectrochemical series, Jahn-Teller distortion; M.O treatment of octahedral complexes. Term symbol, splitting of term by ligands. Rules for electron transition. Orgel diagram for d^1 to d^9 system in octahedral and tetrahedral geometries Charge transfer spectra.

Organometallic Compounds

Definition, classification, Transition metal-to carbon sigma bonded compounds. Synthesis and bonding of Alkyne, Alkene and allyl transition metal complexes, cyclopentadienyl and arene metal complexes, Homogeneous catalysis involving organometallic compounds; Hydrogenation, Polymerization reactions.

ORGANIC CHEMISTRY

IUPAC nomenclature of organic compounds.

Reactive intermediates

Structure & stability of carbocations (Classical & non classical), Carbanions, free radicals, carbenes, nitrenes & arynes.

Stereochemistry: Chirality, planar, central and axial symmetry, configuration systems E & Z configuration, D, L and R & S concept, conformational analysis of six membered ring systems. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Aromaticity: Concept, Huckel rule with examples, Annulenes, benzenoid and non-benzenoid systems. Homoaromaticity and antiaromaticity.

Electrophilic substitution

Theoretical treatment, structure – reactivity relationship in monosubstituted benzene, isomer proportions, orientation in benzene with more than one substituent. Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Pechmann reaction, Fries rearrangement.

Aromatic substitution reactions

Aromatic nucleophilic substitution reactions, general introduction to different mechanisms, structure reactivity relationship, Substitution through diazonium ions.

Addition reactions: Addition to C=C involving electrophile and nucleophiles, general mechanism, orientation and stereochemistry, Addition to cyclopropane, hydroboration. Michael reaction.

Addition to Carbon heteroatom multiple bond: mechanism of nucleophilic addition to Carbon oxygen multiple bond, Mannich reaction, Reformatsky reaction, Tollens reaction, Wittig reactions, Aldol condensation, Cannizzaro's reaction, Perkin reaction, Knoevenagel reaction, benzoin condensation,

Elimination reactions: description of E1, E2, E1cB & E2cB mechanisms, Saytzeff & Hoffman Rule, cleavage of quaternary ammonium hydroxides, conversion of vicinal dihalides to Olefins,

Reaction Mechanism:

SN1 & SN2 mechanisms, Neighboring group participation, Substitution at Allylic & Vinylic, Mechanism of following rearrangements:

Wagner-Meerwein, Pinacolone, Benzil-Benzilic acid, Wolf's, Hoffman, Curtius, Bayer-Villiger & Wittig.

Pericyclic reactions: Cycloadditions, electrocyclic reactions & Sigmatropic rearrangements.

Nuclear Magnetic Resonance Spectroscopy: Nuclear spin, nuclear resonance, saturation, shielding and de-shielding of magnetic nuclei, chemical shifts and its measurements, factors influencing chemical shift, spin-spin interactions, coupling constant 'J' and spin decoupling.

Infrared Spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acid anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect.

Biomolecules: Structure, classification and functional importance of Carbohydrates, Amino Acids, Nucleic Acids.