

DEPARTMENT OF CHEMISTRY
RESTRUCTURED SYLLABUS
Semester I

Physical Chemistry

Thermodynamics I

12

Lectures

- a. Basic concepts and definitions – Applicability of thermodynamics, thermodynamics systems and their classification, Universe, system, surroundings and different types of boundaries
- b. Zeroth law and temperature
- c. Thermometry
- d. Processes, reversible and irreversible process, thermodynamic equilibrium and steady state.
- e. Work and heat involved in a thermodynamic process.
- f. First law and Concept of internal energy
- g. Application to various kinds of processes
- h. State and path functions, exact and inexact differentials
- i. Change in Internal energy
- j. Joule's experiment and consequences
- k. Enthalpy
- l. Specific heat at constant volume and pressure, relationship between them and their differences
- m. Standard states
- n. Kirchoff's equations
- o. Thermo-chemistry

Chemical Kinetics and Catalysis

12

Lectures

- a. Rate of a reaction
- b. Rate laws and rate constants
- c. Order and molecularity
- d. Integrated rate laws
- e. Half-life and its significance
- f. Determination of order of a reaction
- g. Unimolecular reaction and reaction mechanism
- h. Multi-step reactions
- i. Rate-determining step
- j. Zero and fractional order reactions
- k. Steady state approximation and Equilibrium approximation
- l. Rate expression for complex reactions
- m. Molecular reaction dynamics and concept of reactive encounters
- n. Collision theory
- o. Energy and steric requirements (Basic qualitative overview)
- p. Catalysts and inhibitors
- q. Homogeneous catalysis
- r. Arrhenius and van't Hoff complexes
- s. Generalized acid-base catalysis
- t. Identification of homogeneous and heterogeneous catalysis
- u. Activation energy diagrams

Lectures

- a. Assumptions
- b. Expression for average pressure
- c. Arrival to other gas laws
- d. Concept of temperature
- e. Maxwell distribution of molecular velocity and speed (in 1, 2, and 3 dimensions), their derivation, nature and characteristics
- f. Wall collision frequency
- g. Calculation of average quantities
- h. Most probable speed
- i. Energy distribution function, average energy and most probable energy
- j. Principle of equipartition of energy
- k. Maxwell-Boltzmann Distribution
- l. Specific heat of gases
- m. Gaseous collisions
- n. Mean free path
- o. Viscosity of gases
- p. Effect of temperature and pressure on viscosity of ideal gases

Inorganic Chemistry**(A) Atomic Structure**

H-Spectra; Wave mechanical model; de Broglie relation; Heisenberg Uncertainty Principle & its significance; Schrödinger Wave Equation (qualitative approach); Radial and Radial Probability Functions; Angular and angular probability functions (qualitative idea only); s, p and d – type atomic orbital envelope diagrams; nomenclature of atomic orbitals. Exchange energy, Hund's rule, limitations of Auf Bau Principle.

(B) Periodic Table

Modern form of Periodic Table (IUPAC version), Nomenclature of Super-heavy elements ($Z > 100$), screening effect and Slater's rules.

Inert Pair Effect, trends in atomic/ionic size, ionization energy, electronegativity and electron affinity of the s-, p-, d- and f- block elements, ionic potential and diagonal relationship in the Periodic Table. Scales of Electronegativity :Mulliken Scale, Pauling Scale and Alred-Rochow Scale. Variation of electronegativity with bond order and oxidation states.

(C) Radioactivity

Atomic nucleus – nuclear stability, n/p ratio and different modes of decay, nuclear binding energy, nuclear forces, Meson field theory, Nuclear Shell Model (elementary idea) and magic numbers.

Nuclear reactions – nuclear fission, nuclear fusion, spallation and transmutation of elements. Uses of isotopes in Chemistry.

Organic Chemistry**(A) General Introduction and Bonding Features in Organic Molecules (12 lectures)**

DBE, steric effects, inductive effects, bond energy, bond polarity & bond polarizability, bond distance, Resonance, Steric inhibition of resonance, hyperconjugation, bond moment, dipole moment, orbital pictures of ethylene, acetylene, allene, formaldehyde and carbene. Orbital pictures of dienes, enynes, enones, vinylcyanide; π - MO diagrams of butadiene, 1,3,5-

hexatriene, allyl systems, benzene: concepts of HOMO & LUMO ; Aromaticity, Huckel's $(4n+2)$ rule, Frost diagram, anti-aromaticity, Homoaromaticity, application of Huckel's rule to benzenoid and nonbenzenoid compounds. Relative strength of organic Acids-Bases.

(B) Stereochemistry of Acyclic Compounds (12 lectures)

Representation of molecules in Fischer, flying wedge, Saw-horse and Newman projection formulae and their inter-translations. Chirality, elements of Symmetry, simple axis of symmetry, plane of symmetry, centre of symmetry, alternating axis of symmetry. Asymmetry & disymmetry, optical activity, meso/dl, specific rotation, molar rotation. Enantiomerism & Diastereoisomerism, Stereogenic centres involving C=C, C=N, Absolute configuration: D/L, R/S, Relative configuration: E/Z, syn/ anti, cis/trans, erythro/threo, like/unlike nomenclature.

Isomerism involving two like/unlike stereogenic centres (AA and ABA types), pseudoasymmetric centres, stereogenicity, chirotopicity, achirotopicity.

(C) Reaction Mechanism (6 lectures)

Bond Cleavage & Bond Formation- heterolytic & homolytic bond cleavage at stereogenic (single) and non-stereogenic centres, racemization, formation of racemic products. Reactive intermediates: Electrophiles, nucleophiles, radicals. Carbocations (onium and enium ions), carbanions, carbenes; Structure and stability.

Semester II

Physical Chemistry

Thermodynamics II

12

Lectures

- a. Need for the Second Law
- b. Carnot's heat engine and refrigerator
- c. Statements of the second law and their equivalence
- d. Thermodynamic temperature scale
- e. Carnot's theorem
- f. Entropy as a state function
- g. Entropy change of various processes (reversible and irreversible)
- h. Clausius inequality
- i. Combined first and second law
- j. Thermodynamic equation of state
- k. Auxiliary state functions – Gibbs and Helmholtz energies
- l. Maxwell relations
- m. Joule-Thomson experiment
- n. Temperature dependence of Gibbs free energy (Gibbs-Helmholtz equations)
- o. Gibbs free energy of real gases and fugacity
- p. Spontaneity and equilibrium
- q. Gibbs-Helmholtz equation
- r. Concept of chemical potential of pure substances
- s. Partial molar quantities
- t. Gibbs-Duhem equation

Real gases

12

Lectures

- a. Deviation from ideal behaviour with reference to Andrew's and Amagat's experiment, Joule (qualitative idea) and Joule-Thompson experiment (qualitative idea).
- b. Compressibility factor
- c. Concept of attractive and repulsive forces among real gas molecules. Temperature dependence
- d. van der Waal's equation of state
- e. Critical state, critical pressure, volume and temperature, and their form for a van der Waal's gas.
- f. Boyle temperature and their form for a van der Waal's gas.
- g. Brief review of the equation of states (Dieterici).
- h. Virial equation of state, first and second virial coefficient, their relation to other constants and their significance.
- i. Reduced equation of state and the Law of corresponding states
- j. Continuity of states
- k. Nature of intermolecular forces

Quantum Mechanics I

- a. Blackbody radiation, Classical Theory of Rayleigh-Jean, Ultraviolet catastrophe and Planck's theory, Thermodynamic viewpoint
- b. Photoelectric effect, Einstein's Quanta,
- c. Compton effect,

- d. Dual nature of electromagnetic radiation
- e. de Broglie's hypothesis
- f. Wave particle duality
- g. Matter wave
- h. Concept of wave packets
- i. Uncertainty principle, its various mathematical forms and its justifications

Inorganic Chemistry

(A) Ionic Bonding

Packing of ions in crystals, radius ratio rules – applications & limitations; lattice energy – Born-Landé equation and its applications

Born-Haber Cycle and its applications; solvation energy, dissolution of ionic solutes in polar solvents; Polarizability & Fajan's Rules; Stoichiometric and non-stoichiometric defects in crystals (non-mathematical approach), Van der Waal's forces, Hydrogen bonding and its applications.

(B) Coordination Chemistry – I

Double salts, Complex salts, Werner's Coordination Theory, mono- poly- and ambidentate ligands, Chelate complexes, Inner metallic complexes, IUPAC nomenclature of complexes, application of chelates in qualitative and quantitative chemical analysis.

(C) Covalent Bonding – I

Formal Charge, VSEPR theory and structure of inorganic molecules, Berry pseudorotation, hybridization, Bent's rule, dipole moment, resonance.

Organic Chemistry

(A) Energetics of reaction (10L)

Free energy profile for one-step & two-step reaction. Hammond postulate, Kinetically Controlled Vs Thermodynamically Controlled reactions, Investigation of reaction mechanism: Kinetic studies, study of intermediates, cross over experiments, stereochemical proof, isotope labelling- kinetic & non-kinetic, primary kinetic isotopic effect (k_H/k_D) only.

(B) Tautomerism (3L)

Application of thermodynamic principles in tautomeric equilibria [keto-enol tautomerism, composition of the equilibrium in different systems (simple carbonyl, 1,3 and 1,2-dicarbonyl systems, phenols and related system), substituent and solvent effect].

(c) Nucleophilic substitution and elimination reactions (8L)

Nucleophilic substitution and elimination reactions of alkyl halides; S_N1, S_N2, S_Ni, NGP, E1, E2, E1cB mechanisms; Elimination vs Substitution; Saytzeff and Hoffmann rules; reactivity of aryl, vinyl, allyl and benzyl halides.

(D) Stereochemistry of acyclic compounds (14L)

Axial chirality, systems with odd and even number of cumulated double bonds, atropisomerism in biphenyl systems, R/S nomenclature of axially chiral systems. Resolution of racemic acids, bases and alcohols; Optical purity/enantiomeric excess. Topicity of ligands and faces (elementary idea). Homotopic, Enantiotopic & Diastereotopic ligands and faces; prochirality, pro-R, Pro-S, and re/si descriptors.

Conformational Nomenclature- eclipsed, staggered, gauche, anti; dihedral angle, energy barrier of rotation, relative stability of conformers on the basis of steric effects; dipole-dipole interaction, H-bonding; conformational analysis of ethane, propane, n-butane, 1,2-dichloroethane, 2-methylbutane, 1,2-glycols, invertomerism of trialkylamines.

Semester III

Physical Chemistry

Chemical Equilibrium

12

Lectures

- Thermodynamics of mixing of ideal gases
- Conditions of spontaneity and equilibrium in terms of internal energy, Enthalpy, Gibbs and Helmholtz free energy
- Gibbs free energy change of a mixture of gases
- Gibbs free energy change of a reaction
- Definition of molar Gibbs free energy change of a reaction
- Equilibrium in ideal gas mixture and heterogeneous reaction
- Concept of Equilibrium constant, concept of activity and concentration
- Effect of temperature and pressure on equilibrium
- Thermodynamic derivation of van Hoff equation
- Temperature dependence of equilibrium constant and van Hoff isotherm
- Various equilibrium constants and their interrelation
- Temperature dependence of K_c
- Concept of standard state free energy change of a reaction in pressure and concentration scale
- Le Chatelier principle
- Solubility equilibria
- Salt effect
- Nernst distribution law and generalised Distribution equilibrium

Electrochemistry I

12 Lectures

- Activity, ionic activities, mean ionic activities
- Activity coefficient and mean ionic activity coefficient
- Debye-Huckel Limiting law (without derivation)
- Flow of electrical charge through a solution and its consequences
- Specific and equivalent conductance
- Effect of dilution, dielectric constant of solvent, viscosity of solvent and temperature on conductance of strong and weak electrolytes
- Electrophoretic and Asymmetric effect
- Determination of acidity constant of a weak acid: Ostwald dilution law, ionic product of water, determination of ionic radii
- Kohlrausch's law
- Ionic mobilities
- Transport number and its determination (Hittorf's and moving boundary method)
- Effect of concentration and temperature on transport number
- Abnormal transport number
- Transport number in a mixture of two nonreactive electrolytes

Quantum Mechanics II

12

Lectures

- Operators, Linear operators
- Hermitian operators
- Postulates of Quantum Mechanics
- Schrödinger equation
- Solution of Schrödinger equation as wave function and energy (eigenvalues and eigenfunctions)

- f. Commutators and their implication with respect to x, p_x .
- g. Expectation values
- h. Properties of eigenfunctions
- i. Energy quantization
- j. Simple systems: 1-D, 2-D, 3-D box (eigenvalues, eigenfunctions, expectation values, quantum numbers, degeneracy, probability density)
- k. Simple Harmonic Oscillator: Setting the Schrödinger equation, derivation, eigenvalues and eigenfunctions, zero point energy
- l. Tunneling- Basic concepts

Inorganic Chemistry

(A) Redox Equilibrium

Balancing redox reactions by the ion–electron method; Standard redox potential, Nernst equation, influence of pH, precipitation and complexation on redox potential, formal potentials, feasibility of redox titrations, redox potential at equivalent point, redox indicators; redox diagrams – Latimer and Frost diagrams of concerned elements and their applications (typical examples).

(B) Group Chemistry – I : Group 1 and 2

Solutions of alkali metals in liquid ammonia; complexation with crown–ethers, cryptands and related ligands; basic beryllium acetate; detection of metal ions – Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Sr^{2+} , Ba^{2+} in qualitative analysis.

(C) Group Chemistry – II : Groups 13 & 14

General trends in the oxidation states, hydrides, oxides, halides of B, Al, Ga, In, Tl; special features in the chemistry of boron trihalides, diborane, boron nitride and borazine; General trends in the oxidation states, catenation property, hydrides, halides and oxides of C, Si, Ge, Sn, Pb; special features in the chemistry of graphite, fullerenes, silicates, silicones and chlorofluorocarbons; ultra–pure silicon.

(D) Covalent Bonding – I

Molecular orbital theory : Qualitative approach to molecular orbital theory; MO energy level diagrams of H_2 , Li_2 to N_2 , O_2 , F_2 , CO , NO , CN^- , HF , HF_2^- , BeH_2 , CO_2 .

Metallic bonding : qualitative treatment of Band Theory; conductors, semiconductors and insulators.

Organic Chemistry

(A) Aromatic substitution reactions (6L)

Aromatic electrophilic substitution reactions: π -complex, σ -complex, activating and deactivating groups, orienting influence of groups. Aryl halides: activated aromatic nucleophilic substitution, cine substitution. Ipsosubstitution.

(B) Mechanism of free-radical substitution (2L)

Alkane H, allyl/benzyl H; reactivity and selectivity of substitution by chlorine and bromine;

(C) Addition to carbon-carbon multiple bonds (12L)

Reactivity, regioselectivity (Markownikoff's rule), stereoselectivity, chemoselectivity; halogenation, hydrogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, hydroxylation, ozonolysis, carbene addition to alkynes, allenes;

free radical addition to C=C bond, peroxide effect; electrophilic and free radical addition to conjugated dienes; 1,2- vs 1,4-addition; Michael addition; Birch reduction of alkadienes and alkynes; reactions involving alkynic C-H cleavage; Diels-Alder reaction (simple treatment). Interconversion of constitutional isomers of alkene and alkynes, Interconversion of E and Z isomers of alkenes.

D) Spectral Methods in Organic Chemistry- UV & IR and NMR Spectra (15L)

UV-Spectra: Electronic Transitions ($\sigma \rightarrow \sigma^*$, $n \rightarrow \sigma^*$, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$), Relative position of λ_{\max} considering conjugative effect, steric effect, solvent effect, effect of pH, relative intensity of absorption of allowed transitions, bathochromic shift, hypochromic shift, hyperchromic shift, hypsochromic shift with typical examples.

IR-Spectra: Modes of molecular vibrations, application of Hooke's law, Characteristic stretching frequencies of O-H, N-H, C-H, C-D, C=C, C=N, C=O; factors affecting stretching frequencies.

NMR Spectra

Nuclear spin, NMR-active nuclei, principle of PMR, equivalent & non-equivalent protons, anisotropy, chemical shifts, shielding/deshielding protons, upfield & downfield shifts. NMR peak area, relative peak positions of Toluene, nitro-benzene, o, m, p- dichloro- and dinitro-benzenes & chloronitobenzenes; spin-spin coupling in ethanol (ordinary grade), ethyl bromide; 1,1-dibromoethane; 1,2-dibromoethane; 1,1,2-tribromoethane.

Semester IV

Physical Chemistry

Electrochemistry II

12

Lectures

- a. Electrochemical cells
- b. Electrode, electrolyte
- c. Electrode reaction and cell reaction
- d. Nernst equation
- e. Standard electrode potential and application
- f. Formal potential and its application
- g. Thermodynamic functions from cell potential measurement
- h. Concentration cells (with and without transference)
- i. Liquid junction potential, its determination and elimination
- j. Application of e.m.f. measurement (related to practical experiments)

Statistical Mechanics and Reaction Rate Theories

12

Lectures

- a. Energy states and levels
- b. Micro and macro states
- c. Thermodynamic probability
- d. Entropy and probability
- e. Maxwell-Boltzmann statistics
- f. Distribution of molecular states: Boltzmann distribution
- g. Application to Maxwell's velocity distribution and barometric distribution
- h. Partition function and its significance
- i. Translational, rotational and vibrational partition function and their significance
- j. Thermodynamic properties (internal energy, enthalpy, Helmholtz free energy, Gibbs free energy, chemical potential, entropy and value of β)
- k. Reaction coordinate and PES
- l. Transition state theory and activated complex
- m. Expression of rate constant in terms of partition function, the Eyring equation

Liquid and Solid state

12

Lectures

- a. General features of liquid state (short and long range order/disorder, hole theory)
- b. Vapour pressure
- c. Young and Laplace equation
- d. Surface tension
- e. Surface energy
- f. Excess pressure
- g. Capillarity phenomenon
- h. Work of adhesion and cohesion
- i. Contact angle
- j. Spreading of liquids
- k. Dupre equation
- l. Temperature dependence of surface tension
- m. measurement of surface tension
- n. Viscosity of liquids

- o. Temperature dependence of viscosity of liquids
- p. Poiseuille's equation and Measurement of surface viscosity

Solid state

12

Lectures

- a. Types of solids: crystalline state and its properties
- b. Types of crystals
- c. Lattice points
- d. Lattice planes
- e. Unit lattice
- f. Basis
- g. Bravais lattice and its 14 lattice types
- h. Miller indices
- i. X-ray diffraction
- j. Bragg's law
- k. Calculation of basis per unit crystal, volume, density per unit cell
- l. Diffraction techniques (Qualitative treatment only): single crystal and powder
- m. Structure elucidation of NaCl, KCl, CsCl, diamond, graphite and hcp
- q. Specific heat of solids (Dulong Petit law, Einstein theory, Debye correction qualitatively)

Quantum Mechanics III

12

Lectures

- a. Particle on a Ring
- b. Concept of the effective potential
- c. Particle on a sphere: coordinate system
- d. Form of Schrodinger equation in polar coordinates
- e. Form of Schrodinger equation for a two particle system in Cartesian co-ordinates and reduction to one particle system
- f. The diatomic rigid rotor: solution of θ and ϕ part (basic expression only)
- g. Expression of L^2 , L_z in polar coordinate, physical significance
- h. Concept of effective potential
- i. Central force problem and formulation of the Schrodinger equation for hydrogen atom

Colloids, Polymers and Surface Processes

12

Lectures

- a. Colloids: Definition, general properties
- b. Optical properties of colloids
- c. Rayleigh equation and its outcomes
- d. Qualitative understanding of electrokinetic phenomenon: electrophoresis, electroosmosis, streaming potential and sedimentation potential
- e. Electrical double layer, Zeta potential
- f. Mechanism of coagulation
- g. Schulze-Hardy rule
- h. Gold number
- i. Surface excess and Gibbs adsorption isotherm
- j. Surfactant
- k. Critical micellar concentration, its stoichiometric and conductometric determination
- l. Micelles

- m. Thermodynamics of micellization
- n. Liquid crystals
- o. Polymer and degree of polymerization
- p. Molecular weight of polymer (number and weight average molecular weight)
- q. Number distribution and weight distribution function
- r. Expression of number average and weight average molecular weight and their interrelation
- s. Reaction on surfaces - Physisorption and chemisorption
- t. Adsorption isotherms, derivation of Langmuir adsorption isotherm
- u. Mechanism of surface reactions
- v. Derivation of Langmuir adsorption isotherm

Inorganic Chemistry

(A) Definition of acids and bases; solvents

Recapitulation of Arrhenius concept, Bronsted–Lowry definition, solvent system definition, Lux–Flood definition; Relative strength of hydracids, strength of oxoacids, Pauling's rules; HSAB principle, superacids; Solvent properties of water and liquid ammonia; reactions in liquid ammonia.

(B) Acid – Base equilibria

pH (of strong acid/base solution and weak acid/base solution), buffer solution, pH of a buffer solution, Henderson's equation, buffer capacity; salt hydrolysis, pH of salt solutions (salt of strong acid/weak base; strong base/weak acid and weak acid / weak base); indicators, indicator constant, choice of indicators in acid – base titrations.

(C) Solubility equilibria

Solubility product & common ion effect; applications in group analysis – precipitation of sulphides and hydroxides.

(D) Group Chemistry – III : Group 15, 16, 17 and 18

Group 15 : Catenation, oxidation states, trends in the hydrides, halides, and oxides ; special features in the chemistry of hydrazine, hydroxylamine, hydrazoic acid/azides and phosphonitrilic compounds.

Group 16 : Catenation, atomicity, trends in the halides and hydrides; oxides and fluorides of S and Te; special features in the chemistry of the oxoacids of sulphur; Structure and bonding in O_2F_2 , polythiazyl, tetrasulphur tetranitride.

Group 17 : Trends in the Chemistry of oxides, oxoacids and hydracids; special features in the chemistry of interhalogens, polyhalides, pseudohalogens, uses of potassium bromate and potassium hydrogen iodate in quantitative analysis.

Group 18 : Trends in the ionization energy and reactivities of He, Ne, Ar, Kr, Xe; reactivity, structure and bonding in fluorides and oxofluorides of Xe.

Organic Chemistry

A) Alcohols & Ethers (4 lectures)

Relative reactivity of 1° , 2° , and 3° alcohols in reactions via H-O and C-O cleavages; reactions of alcohols as nucleophiles, nucleophilic substitution reactions at carbinol C, S_N1 , dehydration, dehydrogenation, oxidation of alcohols. Reactions of epoxides and ethers via C-

O cleavage, reactions of α -glycols: cyclic ketal/acetal formation, complex formation with H_3BO_3 , oxidative cleavage of glycolic bond.

B) Aldehydes & Ketones (12 Lectures)

Nucleophilic addition to C=O bond: reactivity of carbonyl compounds, relative stability of adducts, formation of acetal, ketal, thioacetal, thioketal, and cyanohydrin, Grignard reaction, $LiAlH_4$ and $NaBH_4$ reductions, electrolytic reductions, reductive coupling, M.P.V reduction, Cannizzaro reaction, Internal Cannizzaro reaction, benzil-benzilic acid rearrangement; nucleophilic addition to α , β -unsaturated carbonyl compounds, reactions of benzoquinones, reactions with derivatives of NH_3 , Wolff-Kishner reduction, Aldol condensation, Claisen condensation, Directed Aldol condensation, Wittig reaction, Acyloin condensation (use of Me_3SiCl)

Mannich reaction, Enamine reaction, Reformatsky reaction, Darzen's reaction, Perkin reaction, Benzoin condensation, Tischenko reaction. Electrophilic substitution at α -position of carbonyl compounds, D-exchange, Nitrosation, halogenation, Haloform reaction, SeO_2 oxidation.

C) Carboxylic Acids & Derivatives (6 lectures)

Nucleophilic substitution reaction at the acyl carbon of acyl halide, anhydride, ester, amide; tetrahedral mechanism, esterification of carboxylic acid and hydrolysis of esters: $A_{Ac}2$, $A_{Ac}1$, $A_{Al}1$, $B_{Ac}2$, $B_{Al}1$, $B_{Al}2$ mechanisms. Reactions via cleavage of α -C-H (use of trimethylsilyl chloride): HVZ reaction, Claisen ester condensation, Bouveault Blanc reduction, decarboxylation, Hunsdiecker reaction, action of heat on hydroxy acids.

Group-II

D) Organometallic compounds and Organonitrogen Compounds (10 lectures)

i) Grignard reagents: Preparation and synthetic applications of Grignard reagents and organolithium compounds. Organocopper compounds: Corey-House, Organocuprates.

ii) Organonitrogen Compounds: Acidity of α -H of nitroalkanes, reduction of aromatic nitro compounds, alkyl cyanides and isocyanides and their hydrolysis, Von Richter reaction. Distinction among 1°, 2°, and 3° amines and their separation, Hofmann's exhaustive methylation, carbylamine reaction, partial reduction of aromatic nitro compounds.

Amines: Ring substitution vs N-substitution in aromatic amines, diazotisation and coupling reactions, synthetic applications of aromatic diazonium compounds. Preparation and synthetic uses of diazomethane and diazoacetic ester.

E) Rearrangement Reactions (8 lectures)

Rearrangements involving electron deficient C, N and O: Allylic rearrangement, Wagner rearrangement, Wolff rearrangement, Arndt-Eistert synthesis, Baeyer-Villiger oxidation, Cumene peroxide-phenol rearrangement, Dakin reaction, Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement, rearrangements of N-azo to C-azo compounds, Orton rearrangement, Hofmann-Martius rearrangement, benzidine rearrangement.

F) Phenols (4 lectures)

Ambident nucleophile, ring substitution Vs O-Substitution. Reactions of phenols: Reimer-Tiemann reaction, Kolbe reaction, Houben-Hoesch reaction alkylation, acylation, Fries rearrangement, Claisen rearrangement, nitration, sulphonation, halogenation,

Physical Chemistry

Semester V

Phase equilibria 12

Lectures

- a. Definition of phase
- b. Phase boundaries
- c. Components
- d. Thermodynamic condition for phase equilibrium
- e. Phase rule and its derivation
- f. Phase equilibrium for one component system (for example H₂O, S, CO₂)
- g. First and second order phase transition
- h. Clapeyron equation
- i. Clausius-Clapeyron equation
- j. Trouton's rule
- k. Liquid-vapour equilibrium for two component system
- l. Review of the Gibbs-Duhem and the Duhem-Margules equation
- m. Constant boiling mixture
- n. Critical solution temperature
- o. Completely immiscible systems
- p. Thermodynamics of mixing of binary solutions
- q. Simple eutectic systems

Spectroscopy I 12

Lectures

- a. Spectroscopy - Nature of electromagnetic radiation, range of wavelength
- b. Transition moment integral (qualitative idea) and allowed transitions
- c. Separation of electronic and nuclear motion – Born-Oppenheimer approximation
- d. Signal to noise ratio
- e. Width and intensity of transition, line broadening
- Rotational spectroscopy
- f. Rigid rotor (diatomic only)
- g. Selection rule
- h. Spectrum: position and intensity of spectral lines.
- i. Non-rigid rotor and its effect on energy levels
- j. Selection rule and spectrum
- k. Application
- l. Isotope effect

Atomic Structure and Atomic Spectra 12

Lectures

- a. Appropriate treatment of Schrödinger equation for Hydrogenic system
- b. Solution of radial, θ and ϕ part (General expression)
- c. Shapes of s, p, d orbitals
- d. Hydrogenic wave functions up to $n=3$
- e. Atomic orbitals and their energies
- f. Spectroscopic transitions and selection rules.
- g. Concept of electronic spin
- h. Spectra of complex atoms - singlet and triplet states
- i. Spin-orbit coupling and fine structure
- j. Term-Symbol and LS coupling

Inorganic Chemistry

(A) Isomerism, Reactivity and Stability of coordination complexes

Constitutional, Geometrical and optical isomerism with respect to C.N. = 4 and 6; Mills and Quibell complex, examples of purely inorganic optically active complexes; labile and inert complexes; substitution in square planar complexes and trans – effect (examples and applications); choice of ligands and stability of various oxidation states of the 3d metal ions; stability constant of complexes.

(B) Structure and Bonding in coordination complexes

VBT, CFT, splitting of d^n configurations in octahedral and tetrahedral fields, crystal field stabilization energy in weak and strong fields, pairing energy, Jahn – Teller distortion and its application; MOT (elementary idea), sigma and pi – bonding in octahedral complexes (a pictorial approach)

(C) Organometallic Chemistry

18 electron rule and its application to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, metal–carbon sigma and pi – bonded organometallic complexes of transition metals; bonding and IR spectra of carbonyls and nitrosyls; Zeise's salt – its preparation properties and structure; ferrocene – its preparation, properties and structure; elementary idea of fluxional molecules; oxidative addition, reductive elimination and insertion reactions; homogenous catalysis of organometallic compounds – hydrogenation, hydroformylation, and polymerization of alkenes (Ziegler – Natta catalyst)

Organic Chemistry

A) Synthetic strategies and asymmetric synthesis (14 lectures)

Disconnection approach towards synthesis of bifunctional molecules (both cyclic and acyclic): concepts of synthons, synthetic equivalents (ethyl acetoacetate, ethyl cyano acetate and diethyl malonate as examples). Functional group interconversion (FGI). Protection and deprotection of common functional groups (-OH, carbonyl, -NH₂, -CO₂H) in synthetic route, activation of synthetic equivalents. Umpolung: Illogical electrophiles and nucleophiles. Disconnection and synthesis of 1,3; 1,4 and 1,5-dioxygenated compounds. Robinson ring annulation, applications of Claisen rearrangement, Favorskii rearrangement and Demjanov rearrangements involving electron deficient C, O, N. Large ring synthesis: High dilution techniques. Asymmetric synthesis:

B) Pericyclic reactions (8 lectures)

Definition and classification. Electrocyclic reactions: FMO approach, examples of electrocyclic reactions (thermal and photochemical) involving 4 and 6 π -electrons and corresponding cycloreversion reactions. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2 + 2] reactions. Sigmatropic shifts and their order. [1,3] and [1,5] H-shifts. [3,3]-shifts with reference to Claisen and Cope rearrangements.

C) Stereochemistry of alicyclic compounds and Dynamic stereochemistry (12 lectures)

Stereoisomerism of di-substituted ring compounds, ring size strain and Baeyer strain theory, concept of I-strain. Conformational analysis of cyclohexanes: energy profile of ring inversion of cyclohexane, symmetry properties of chair, boat and skew-boat conformations, conformational analysis of mono- and di-substituted cyclohexanes. E2, S_N2 and NGP,

lactonisation reactions of cyclohexane systems, oxidation of cyclohexanols with chromic acid, pinacol-pinacolone rearrangements, esterification, saponification of esters, steric assistance and steric hindrance.

Analytical Chemistry

[33L] UNIT 1:

CONVENTIONAL METHODS OF ANALYSIS

15L

- (a) Redox Titrimetric analysis of Fe, Cu, Zn, Cr, Mn. Formol titration, estimation of sugars and vitamin C (principles only).
- (b) Complexometric Titrations – Metal ion indicators, masking, demask agents (examples). Principles for the estimation of (Ca + Mg), (Fe + Al), and (Cu + Zn) in a mixture of complexometry.
- (c) Basic concepts and simple application of chromatography – Thin layer, paper and column chromatography, R_f -values. Ion exchange chromatography (IEC): Ion exchange resins and their ion exchange capacities, deionization of water. Solvent extraction: Definition, types, principle and efficiency; factors affecting extraction, extraction with a metal chelator, gas chromatography, HPLC, extraction with dithiozone.

UNIT 2: INSTRUMENTAL METHODS OF ANALYSIS

10L

- (a) Flame Spectrometry – Introduction, Principles, Elementary Theory and Instrumentation of atomic absorption and atomic emission spectrometry; Determination of Ca and Mg in tap water (application).
- (b) Radiochemical methods and Environmental analysis. Basic instrumentation, Measurement of radioactivity, Neutron activation analysis, Isotope dilution analysis, radiometric titrations, hazards of radiation and safety measures.

UNIT 3: ERROR ANALYSIS AND ANALYSIS OF SAMPLES

8L

- (a) Error Analysis – Errors and their classifications, determinate and indeterminate errors, systematic and random errors, accuracy and precision, distribution of random errors; statistical analysis of data; methods of least squares and standard deviation, confidence interval, significance testing

Semester VI

Physical Chemistry

**Thermodynamics III
Lectures**

12

- a. The Nernst heat theorem
- b. Third law of thermodynamics
- c. Residual entropy
- d. Raoult's law
- e. Henry's Law
- f. Positive and negative deviation from ideal behaviour
- g. Ideal solution and ideally dilute solution
- h. Definition and thermodynamic origin of colligative properties
- i. Thermodynamic derivation of colligative properties of solution using chemical potential and their interrelationships (lowering of vapour pressure, depression of freezing point, elevation of boiling point and osmotic pressure)
- j. Abnormal colligative properties

Spectroscopy II

12

Lectures

- a. Vibration of a diatomic molecule and simple harmonic oscillator
- b. Review of solution of quantum harmonic oscillator (general expression)
- c. Selection rule for harmonic oscillator
- d. Spectrum
- e. Anharmonicity and its effect on energy levels
- f. Selection rule for anharmonic oscillator
- g. Vibrational spectrum
- h. Rotational – vibrational coupling in the limit of Born-Oppenheimer approximation
- i. Raman spectroscopy (Qualitative)
- j. Rayleigh and Raman scattering
- k. Polarizability ellipsoids
- l. Features and condition for Raman activity (for linear and non-linear AB₂ molecule)
- m. Rotational and vibrational Raman spectra and its characteristics

Photochemistry

12

Lectures

- a. Potential energy curves for electronic states, Frank-Condon principle
- b. Decay of excited states by radiative and non-radiative paths
- c. Timescales
- d. Fluorescence and phosphorescence
- e. Jablonski diagram
Mechanism of relaxation through non-radiative paths (Unimolecular and bimolecular mechanism (collision, energy transfer))
- f. Photophysics of the excited state
- g. Laws of photochemistry
- h. Quantum yield and its measurement for photochemical processes
- i. Photo-stationary state
- j. Photosensitized reactions
- k. Photochemistry of Photosynthesis

Inorganic Chemistry

(A) Magnetism and Spectra of Coordination Complexes

Orbital and spin magnetic moments, spin only magnetic moments of 3dⁿ ions and their correlation with effective magnetic moments, quenching of magnetic moments in presence of

crystal field; ferromagnetic and anti-ferromagnetic coupling (elementary idea with examples only); d-d spectra, weak-field splitting schemes, qualitative Orgel diagrams for d^n systems and their spectroscopic ground states, selection rules for spectral transitions, charge transfer spectra (elementary idea with examples only).

(B) Bioinorganic Chemistry

Essential and trace elements of life; role of metal ions in biology – Na^+ , K^+ , Ca^{2+} , Mg^{2+} , $\text{Fe}^{2+/3+}$, Cu^{+2+} , Zn^{2+} ; active site structures and bio-functions of myoglobin, haemoglobin, cytochromes, ferredoxins, carbonic anhydrase; photosynthesis – PS-I and PS-II, sodium ion pump and ionophores, metal ion induced toxicity and chelation therapy, metal ion as drugs (cisplatin and a few gold drugs)

(C) Chemistry of the Lanthanides

General characteristic with respect to electronic configuration, oxidation states and ionization enthalpies, lanthanide contraction, separation of lanthanides by ion-exchange method.

Organic Chemistry

A) Heterocyclic compounds (12 lectures)

Synthesis (including retrosynthetic approach), Knorrpyrrole synthesis, Hantz pyridine synthesis, Fischer indole synthesis, Skraup's quinoline synthesis, Bischler-Napieralski synthesis, reactivity, orientation and important reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline, and isoquinoline.

B) Carbohydrates (10 lectures)

Monosaccharides- classification, osazone formation, stepping up and stepping down of aldoses, interconversion of aldoses to ketoses and vice versa, epimerisation. Constitution and configuration of D-glucose and D-fructose, ring structure and conformational aspects of D-glucose and its derivatives, anomeric effect, mutarotation of D-glucose. Disaccharides: structure of sucrose.

C) Amino acids (10 lectures)

Synthesis of α -amino acids (Gabriel, Strecker, azlactone, acetamido, malonic ester methodologies). Isoelectric point, ninhydrin reaction, resolution of amino acids. Peptides: geometry of peptide linkage, peptide synthesis including Merrifield synthesis, structure determination of peptides, C-terminal and N-terminal unit determination, determination of amino acid sequence.

Biochemistry

A) Structural aspects of Biomolecules

9 lectures

Proteins- Introduction and classification. Protein structure- primary, secondary, tertiary and quaternary structure (Forces that stabilize structure of proteins: H-bonds, hydrophobic bond, electrostatic attraction, Vanderwaals interaction, dipole-dipole interaction.) Denaturation and renaturation of proteins. Behavior of proteins in solutions, salting-in and salting-out of proteins. Structure and biological function of fibrous proteins (keratins, collagen and elastin)

*(Globular proteins and structural aspects of carbohydrates are excluded as Chem (H) students study these in details in Bioinorganic Chemistry).

Nucleic acids- Nucleosides and nucleotides. Nature of genetic material. Composition of RNA and DNA, generalized structural plan of nucleic acids, nomenclature used in writing structure of nucleic acids, complementary base-pairings, features of DNA double helix (Watson-Crick model). Denaturation and annealing of DNA, structure and role of different types of RNA. Size of DNA of prokaryotic and eukaryotic cells.

Lipids- Definition and classification. Fatty acids- properties of saturated and unsaturated fatty acids. Esters of fatty acids-formation and hydrolysis; Essential fatty acids. Triacylglycerols. Reactions and characterization of fats – hydrolysis, saponification value, iodine number, rancidity of fats, Reichert- Meissel number. Biological significance of fats. Characterization of fats, Phospholipids, Micelle bilayer, liposomes, Glycolipids, steroids and sterols.

- B) Bioenergetics and Metabolism: (2.5 marks) 2 lectures**
Principles of Bioenergetics: Bioenergetics and Thermodynamics, Phosphoryl group transfers and ATP generation, Biological Oxidation and Reduction reaction.
- C) Carbohydrate metabolism: (5 marks) 5 lectures**
Intracellular metabolism of glucose - glycolysis, reaction and energetic of TCA cycle, (gluconeogenesis, glycogenesis, glycogenolysis, reactions and physiological significance of pentose phosphate pathway, regulation of glycolysis, TCA cycle, and glycogen metabolism).
- D) Oxidative phosphorylation and electron transport chain: (2.5 marks) 2 lectures**
Structure of mitochondria, sequence of electron carriers, ATP synthesis, inhibitors of ETC, basic concept of oxidative phosphorylation, inhibitors and uncouplers of oxidative phosphorylation, photophosphorylation.
- E) Lipid metabolism: (2.5 marks)**
Metabolism (anabolism and catabolism) of triglyceride, Transport of fatty acid into mitochondria, Beta-oxidation of fatty acids, reactions and energetic of beta oxidation, biosynthesis of saturated and unsaturated fatty acids, metabolism of ketone bodies, biosynthesis of phospholipids and cholesterol.
- F) Amino acid metabolism: (5 marks)**
General reactions of amino acid metabolism (oxidative deamination, transamination, decarboxylation etc), glucogenic and ketogenic amino acids, urea cycle, biosynthesis and catabolism of amino acids (glycine, phenylalanine, glutamic acid), inborn errors of amino acid metabolism.
- G) Nucleotide metabolism: (2.5 marks)**
Biosynthesis and catabolism of purines and pyrimidines (Adenine and cytosine)
- H) Enzymes: (20 marks)**
Cofactors – Definition, examples of a) metal ions b) coenzymes c) prosthetic group
Definition, examples of holoenzymes, Apoenzyme.
Classification of enzymes, IUPAC system, Name & examples of each class
Mechanism of enzyme activity—standard free energy change in a reaction-transition

state, activation energy both in non-enzymatic and enzymatic reaction, reaction rate, rate

constant, rate limiting step, rate equation, binding energy, specificity of enzymes geometric and stereo specificity with example, lock & key hypothesis, induced fit hypothesis, proximity and orientation effect, strain and distortion theory, enzyme catalysis-i) acid- base catalysis, ii)metal ion catalysis iii) covalent catalysis – Examples .

Regulatory enzyme- allosteric enzyme, definition & example, allosteric modulators, feedback inhibition, kinetic properties of allosteric enzyme, K enzymes, M enzymes, sequential model & symmetry model, examples, regulation by covalent modification (likephosphorylation), example, regulation by proteolytic cleavage of protein, zymogens,example

Isozymes-Definition and basis of difference, example-lactate dehydrogenase.