Stereochernistry and Bonding in Main Group Compounds
Valence shell electron pair repulsion (VSEPR) theory and its applications, Walsh diagram (triatomic and penta-atomic molecules), dspn bond, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules such as Atomic inversion, Berry pseudorotation, Nucleophilic displacement, free radical mechanisms.

Unit II
Metal-Ligand bonding
Limitation of crystal field Theory, Jahn-Teller effect, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes.

Unit III
Metal-Ligand Equilibrium in Solution
Stepwise and overall formation constants and their relationship, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, Chelate effect and its thermodynamic origin, determination of binary formation constants by pHmetry and Spectrometry.

Unit IV
Reaction Mechanism of Transition Metal Complexes-I
Energy Profile of a reaction, reactivity of metal complex, inert and labile complexes, Kinetic application of valence bond and crystal field theories. Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anion reactions, reactions without metal-ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of substitution reaction.

Unit V
Reaction Mechanism of Transition Metal Complexes-II and HSAB theory
Redox reaction, Electron transfer reaction, mechanism of one electron transfer reactions, outer and inner sphere type reactions, cross reactions and Marcus-Hush theory, HSAB principle, theoretical basis of hardness and softness, Lewis-acid base reactivity approximation; donor acceptor numbers, E and C equation; applications of HSAB concept.

BOOKS SUGGESTED:

2. Inorganic Chemistry, J E. Huheey, Harpers & Row.
Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzoid compounds, alternate and non-alternate hydrocarbons. Hückel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, catenanes and rotaxanes.

Stereochemistry

Strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, three and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Conformational analysis and linear free energy relationship

Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.

Reaction Mechanism: Structure and Reactivity

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects.

Aliphatic Nucleophilic Substitution

The SN2, SN1 mixed SN1 and SN2 and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance.
Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Book Suggested

9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India

Paper-III
MCH-403: PHYSICAL CHEMISTRY I

Unit-I
Introduction to Exact Quantum Mechanical Results
Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.

Unit-II
Approximate Methods
The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Molecular Orbital Theory
Huckel theory of conjugated systems bond and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Huckel theory.
UNIT III

Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum operator using ladder operators addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

Unit-IV

Classical Thermodynamics


Unit-V

Statistical Thermodynamics


Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
4. Coulson’s Valence, R. Mc Weary, ELBS.
Paper-IV
MCH-404: Group Theory & Spectroscopy I

Unit-I
Symmetry and Group theory in Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schoenflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.

Unit-II
Microwave Spectroscopy
Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. applications.

Unit-III
Infrared-Spectroscopy
Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations; normal co-ordinate analysis.

Unit-IV
Raman Spectroscopy
Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).

Unit-V
Electronic Spectroscopy
Molecular Spectroscopy
Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Photoelectron Spectroscopy
Basic principles; photo-electric effect, ionization process, Koopman's theorem
Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.
Auger electron spectroscopy-basic idea.

Books suggested


Paper-V

MCH-405 (a) : MATHEMATICS FOR CHEMISTS
(For students without Mathematics in B.Sc.)

Unit-I

Vectors
- Vector, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

Matrix Algebra
- Addition and multiplication; inverse, adjoint and transpose of matrices.

Differential Calculus
- Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr’s radius and most probable velocity from Maxwell’s distribution etc.).

Unit-II

Integral calculus
- Basic rules for integration, integration by parts, partial fractions and substitution.
- Reduction formulae, applications of integral calculus.
- Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).
Unit-IV

Elementary Differential equations
First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Unit-V

Permutation and Probability
Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting including least squares fit etc with a general polynomial fit.

Book Suggested

1. The chemistry Mathematics Book, E. Steiner, Oxford University Press.

Paper-V

CH-405 (b) BIOLOGY FOR CHEMISTS
(For students without Biology in B.Sc.)

Unit-I

Cell Structure and Functions

Unit-II

Carbohydrates
Unit-III

Lipid
Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.
Lipoproteins—composition and function, role in atherosclerosis. Properties of lipid aggregates—micelles, bilayers, liposomes and their possible biological functions.

Unit-IV

Amino-acids, Peptides and Proteins
Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing.

Unit-V

Nucleic Acids
Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Book Suggested