Inorganic Chemistry-I
CHE-101

Unit-I
Stereochemistry and Bonding in Main Group Compounds:

Valence shell electron pair repulsion (VSEPR) theory and its applications, Walsh diagram (triatomic molecules), dЛ-pЛ bond, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules.

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 constant, 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 potentiometric and spectrophotometry.

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 favor of conjugate mechanism, anion reactions, reactions without metal ligand bond cleavage. Substitution reaction in square planer complexes, the trans effect, Mechanism of substitution reactions.

Unit-V

Reaction Mechanism of Transition Metal Complexes - II and HSAB theory :

Redox reaction, Electron transfer reaction, mechanism of one electron transfer reaction, 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; donar acceptor numbers, E and C equation : applications of HSAB concept.

Books suggested:

1. Advanced Inorganic Chemistry, F. A. Cotton and Wilkinson, John Wiley.

2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.

3. Chemistry of Elements. N. N. Greenwood and A. Earnshow, Pergamon

4. Inorganic Electronic Spectroscopy, A.B. P. Lever, Elsevier.

5. Comprehensive Co-ordination Chemistry eds., G. Wilkinson, R.D. Gillars and J. A. Mc clevetry, Pergamon.

6. Inorganic Chemistry, D. F. Shriver & P.W. Atkins, Oxford University Press 3rd 1999.

7. Inorganic Chemistry by A.G.Sharpe. Addition Wesley England 3rd 1992

8. Inorganic Chemistry G.L.Misseler and D. A. Tarr Pearson Education, 2009.

ORGANIC CHEMISTRY-I
CHE-102

Unit-I

Nature of Bonding in Organic Molecules:

Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, Energy level of -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, and crypt ands, inclusion compounds, catenae's and rotaxanes.

Unit - II

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

Unit - III

Conformational analysis and Linear free energy relationship: Conformational analysis of cycloalkanes, declines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocation's, car anions, free radicals, carbines and interns. The Hammett equation and Linear free energy relationship, substituents and reaction constants, Taft equation.

Unit - IV

Reaction Mechanism : Structure and Reactivity: Types of mechanism, 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, isotopic effects.

Unit - V

Aliphatic Nucleophilic Substitutions: The SN2, SN1, mixed SN1 and SN2 and SEI mechanism. The neighbouring group mechanism. Neighboring group participation by pi and sigma bonds, anchimeric assistance**.** Classical and non classical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements,Carbocations. The SNi mechanism. Nucleophilic substitution at an allylic, trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambient nucleophiles, regioselectivity.

Book Suggested :

1. Advanced Organic Chemistry - Reactions, Mechanism and Structure, Jerry March, John Wiley.

2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.

3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.

4. Structure and Mechanism in Organic Chemistry,_C.K. Ingold, Comell University Press.

5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice - Hall.

6. Modern Organic Reactions, HO. House, Benjamin.

7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blaclcie Academic & Professionls.

Physical Chemistry –I
CHE103

Unit - I

Introduction to Exact Quantum Mechanical Results: Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger 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 non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

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

Unit - III

Angular Momentum: Ordinary Angular Momentum, generalized angular momentum, Eigen functions for Angular Momentum, eigenvalues of Angular Momentum, operator using ladder operators addition of angular momenta, spin, ant symmetry and Pauli exclusion principle.

Unit - IV

Classical Thermodynamics: Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, Partial molar volume and Partial molar heat content and their significance, Determinations of their quantities. Consents of fugacity and determination of fugacity. Non ideal systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transition.

Unit - V

Statistical Thermodynamics: Concept of distribution, thermodynamics probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles. Corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions. Calculation of thermodynamics probability in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and application to metal. Bose-Einstein statistics distribution Law and application to helium.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.

2. Introduction to Quantum Chemistry, A.K. Chandra. Tata Mc Graw Hill.

3. Quantum Chemistry, Ira N. Levine, Prentice Hall.

4. Couison's Valence, R.Mc Weepy, ELBS.

5. Chemical Kinetic. K. J. Laidler, MoGraw-Hill.

6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Milian.

7. Micelies, Theoretical and Applied Aspects V.MOraoi, Plenum.

8. Modern Electrochemistry Vol. 1 and Vol. ll J.O.M Bockris and A.K.N. Reddy, Planum.

9. Introduction to Polymer Science V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Bastern.

10. Introduction to Quamum Chemistry-R.K. Prasad New Age Publication.

GROUP THEORY AND SPECTROSCOPY-I
CHE104

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 Cn,Cnv,Cnh, and Dnh 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 C2v and C3v point group Symmetry aspects of molecular vibrations of H20 molecule.

Unit - II

Microwave Spectroscopy: Electromagnetic spectrum, Quantization of energy, Interaction of electromagnetic radiation with molecular system, Doppler broadening. Pure rotational Spectra: Instrumentation, rigid rotator model, effect of isotopic substitution on the transition frequencies, non-rigid rotator model, Stark effect, Application of rotational spectra to the calculation of bond length of diatomic molecules.

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 vibration, normal co-ordination analysis.

Unit-iv

Raman-spectroscopy: Classical and quantum theories of Raman effect. Vibration 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 level, molecular orbitals, vibronic transition, vibrational progressions and geometry of the excited sates, Franck-Condon principle ,electronic spectra of polyatomic molecules. Emission spectra, radioactive and non-radioactive decay.

Photoelectron Spectroscopy

Basic principles: photo-electric effect, ionization process ,Koopmans's theorem. Photoelectron spectra of simple molecules.

Books suggested:

1. Modern Spectroscopy, .l.M. Hollas, John Viley.

2. Applied Electron Spectroscopy for chemical analysis d. H.

Windawi and FL. Ho, Wiley Interscience.

3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic

Chemistry, R,V. Parish, Ellis Harwood.

4. Physical Methods in Chemistry, R.S. Drago, Saunders College.

5. Chemical Applications of Group Theory, F .A. Cotton.

Mathematics for chemist [Optional]
CHE105 A

Unit –I
Vectors: Vectors, dot, cross and triple products etc. gradient, divergence and curl, vector Calculus.
Matrix Algebra: Addition and multiplication; inverse, adjoin and transpose of matrices.

Unit –II
Differential Calculus: Functions, continuity and differentiability, rules for differentiation, application 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-III
Integral calculus : Basic rules for integration, integration by parts, partial fractions and substitution, Reduction formulae, application of integral calculus, Functions of several variables, partial differentiation, co-ordinate transformation (e.g. Cartesian to Spherical polar).

Unit-IV
Elementary Differential equations : First-order and first degree differential equations, homogenous, exact and liner equations Applications to chemical kinetics , Secular equilibrium, quantum chemistry etc., second order differential equation and their solutions.

Unit-V
Permutation and Probability :Permutation 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.
2. Mathematics for chemistry, Doggett and Suiclific, Logman,
3. Mathematics for physical Chemistry: Daniels, Mc. Graw Hill.

BIOLOGY FOR CHEMISTS (Optional)
CHE105B

Unit –I

Cell Structure and functions: Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animals cells. Over for view and their functions, comparison of plant and animals cells. Overview of metabolic processes-catabolism and anabolism. ATP- the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building of bio-macromolecules.

Unit- II

Carbohydrates: Conformation of monosaccharide's structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, my inositol, amino sugars, N- acetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological functions of glucosminoglyscans of mucopolysaccharides Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition, Blood group substance. Ascorbic acid.

Unit-III

Lipid: Fatty acids, essential fatty acids, structure and functions of triacylglycerol's, glycerophospholipids, Spingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure . lipid metabolism b-oxidation of fatty acids.

Unit-IV

Amino- acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, Secondary Structure of proteins. Force responsible for holding of secondary structures. A- helix, b-sheets super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure, quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acid, sequence determination : chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormones (TRH)

Unit V

Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via Bounding 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, and overview of replication of DNA, transcription, translation and genetic code, chemicals synthesis of mono and trinucleoside

Book Suggested

1. Principles of Biochemistry , A.L. Lehninger, Worth Publisher.
2. Biochemistry, L. Stryer, W.H. Freeman,
3. Biochemistry, J. David Rawan Neli. Patterson.
4. Biolchemistry, Voet and Voet, John Wiley \
5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley