

# NIMS UNIVERSITY, JAIPUR



## SYLLABUS

**M. Sc. CHEMISTRY PREVIOUS**

**M.Sc. (PREVIOUS)****YEAR - I**

<b>Subject</b>	<b>Theory</b>	<b>Practical</b>	<b>Total</b>
Inorganic Chemistry	70	30	100
Organic Chemistry	70	30	100
Physical Chemistry	70	30	100
Group Theory and Spectroscopy	100	-	100
Mathematics for Chemists	100	-	100
Biology for Chemists	100	-	100
Computers for Chemists	70	30	100

## PAPER-I: INORGANIC CHEMISTRY

### UNIT-I

#### **Stereochemistry and Bonding in Main Group Compounds:**

VSEPR, Walsh diagram (triatomic (AH<sub>2</sub> type) and penta-atomic (CH<sub>3</sub>I) molecules), dp- $\pi$  bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

#### **Metal-Ligand Equilibria in Solution:**

Stepwise and overall formation constants and their interaction, 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 pH-metry and spectrophotometry.

### UNIT-II

#### **Reaction Mechanism of Transition Metal Complexes:**

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, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

### UNIT-III

#### **Metal-Ligand bonding:**

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes,  $\pi$ -bonding and molecular orbital theory.

### UNIT-IV

#### **Electronic Spectra and Magnetic Properties of Transition Metal Complexes:**

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d<sup>1</sup>-d<sup>9</sup> states), calculations of  $d$ ,  $B$  and  $b$  parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

### UNIT-V

#### **Metal P-Complexes:**

Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

### UNIT-VI

#### **Metal Clusters:**

Higher boranes, carbonanes, metalloboranes and metallocarbonanes compounds with metal-metal multiple bonds.

#### **Isopoly and Heteropoly Acids and Salts.**

## PAPER-II: ORGANIC CHEMISTRY

### UNIT-I

#### **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. Huckel's rule, energy. Level of p-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 :**

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

### UNIT-II

#### **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, isotope effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity, resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants, Arrhenius equation.

#### **Aliphatic Nucleophilic Substitution:**

The S<sub>N</sub>2, S<sub>N</sub>1 mixed S<sub>N</sub>1 and S<sub>N</sub>2 and SET mechanism. The neighbouring group mechanism, neighbouring 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 S<sub>N</sub>1 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.

**UNIT-III****Aliphatic Electrophilic Substitution:**

Bimolecular mechanisms S<sub>E</sub>2 and S<sub>E</sub>1, The S<sub>E</sub>1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving groups and the solvent polarity on the reactivity.

**Aromatic Electrophilic Substitution:**

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction

**UNIT-IV****Aromatic Nucleophilic Substitution:**

The S<sub>N</sub>Ar S<sub>N</sub>1, benzyne and S<sub>N</sub>1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser, and Smiles rearrangements.

**Free Radical Reactions:**

types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**UNIT-V****Addition to Carbon-Carbon Multiple Bonds:**

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

**Addition to Carbon-Hetero Multiple bonds:**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

**Elimination Reactions:**

The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

**UNIT-VI****Pericyclic Reactions:**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-

hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlatino diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions,  $4n$   $4n+2$  and allyl systems. Cycloadditions-antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes,  $1,3$  dipolar cycloadditions and cheleotrpc reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties,  $3,3$ - and  $5,5$  sigmatropic rearrangements. Claise n, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

**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, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & \* Professionsl.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.

## PAPER-III: PHYSICAL CHEMISTRY

### UNIT-I

#### Quantum Chemistry :-

##### **A. Introduction to Exact Quantum Mechanical Results:**

the 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.

##### **B. 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.

##### **C. 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.

##### **D. 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-II

#### Thermodynamic:-

**A. 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 these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient for electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

**B. Statistical Thermodynamics:**

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

**C. Non Equilibrium Thermodynamics:**

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

**UNIT-III****Chemical Dynamics:**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogeneous catalysis, kinetics of enzyme reactions, general features for fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories for unimolecular reactions).

**UNIT-IV****Surface Chemistry:-****A. Adsorption:**

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs

adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

### **B. Micelles:**

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

## **UNIT-V**

### **Macromolecules:**

Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

## **UNIT-VI**

### **Electrochemistry:**

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Grahman Devanatham-Mottwatts, Tobin, Bockris, Devanathan models, Overpotentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkone equation; half wave potential and its significance.

### **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. Coulson's Valence, R.Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol II 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 Eastern.

## PAPER-IV: GROUP THEORY, SPECTROSCOPY AND DIFFRACTION METHODS

### UNIT-I

#### **Symmetry and Group theory in Chemistry:**

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the  $C_N$ ,  $C_{NV}$ , etc, 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

#### **Unifying Principles:**

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines.

#### **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

#### **Vibrational Spectroscopy:-**

##### **A. 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.

##### **B. 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-IV****Electronic Spectroscopy:-****A. Atomic Spectroscopy:**

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

**B. 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; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

**C. 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.

**UNIT-V****Magnetic Resonance Spectroscopy:-****A. Nuclear Magnetic Resonance Spectroscopy:**

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "J" Classification (AXB, AMX, ABC, A2B2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton-<sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P. FT NMR, advantages of FT NMR.

**B. Electron Spin Resonance Spectroscopy:**

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyper fine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

**UNIT-VI****X-ray Diffraction:**

Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

**Electron Diffraction:**

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces. **Neutron Diffraction:**

Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cell.

**BOOKS SUGGESTED:-**

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. 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.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, harper & Row.

## MATHEMATICS OF CHEMISTS

### UNIT-I

#### **Vectors and Matrix Algebra:-**

##### **A. Vectors:**

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

##### **B. Matrix Algebra:**

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, Skey-Harmitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces, matrix eigenvalues and digenvetors, diagonalization, determinatnts (examples from Juckel theory).

### UNIT-II

#### **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.).

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-III

#### **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.

#### **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.
2. Mathematifs for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistery, J.R. Barante, Prenice Hall.
6. Basic Matchematics for Chemists, Tebbutt, Wiley.

## PAPER-V

### BIOLOGY FOR CHEMISTS

#### UNIT-I

##### **Cell Structure and Functions:**

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal 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 biomolecules, building blocks of biological macromolecules.

##### **Carbohydrates:**

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism-Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

#### UNIT-II

##### **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. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism- $\beta$ -oxidation of fatty acids.

##### **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.  $\alpha$ -helix,  $\beta$ -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 acids, sequence determination : chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

#### UNIT-III

**Nucleic Acids:**

Purine and pyrimidine bases of nucleic acids, base pairing via Hbonding. 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:-**

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

## PAPER-VI COMPUTERS FOR CHEMISTS

**UNIT-I****Introduction to Computers and Computing 8 Hrs.**

Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Algorithms and flow-charts.

**UNIT-II****Computer Programming in FORTRAN/C/BASIC:**

(the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Terminating statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)

**UNIT-III****Programming in Chemistry:**

Developing of small computer codes (FORTRAN/C/BASIC) involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity and Molality of solutions. Evaluation

Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles, dihedral angles, etc.

#### **UNIT-IV**

##### **Use of Computer programmes 15 Hrs.**

Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory. Introduction of working of any one of the packages such as LOTUS/EXCEL/FOXPRO/MOPAC and Word Processing software such as WORDSTAR/MS WORD.

##### **BOOK SUGGESTED:**

1. Fundamentals of Computer: V. Rajaraman (Prentice Hall)
2. Computers in Chemistry: K.V. Raman (Tata Mc Graw Hill)
3. Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)