M.Sc III Semester

Chemistry

Paper-1 Photochemistry (Compulsory farall branches) 60Hrs.

1-Basic of Photochemistry

Absorption, excitation, photochemical laws, quantum yield, electronically excited states- life times-measurements of the times. Flash photolysis, stopped Flow techniques, Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

2- Photochemical Reactions

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molectule, quantum, yield, transfer of excitation energy, actinometry.

3- Properties of Excited States

Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Bimolecular deactivation-quenching.

4- Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical-photo-dissociation, gas-phase photolysis.

5- Photochemistry of Alkenes

Intromolecular reactions of the olefinic bond-geometrical isomerism, cyclisat ion reactions, rearrangement of 1,4 and 1,5-dienes,

6- Photochemistry of Carbonyl compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, β , γ - unsaturated and α,β , unsaturated compounds, Cyclohexadienones. Intermolecular …….....buchi Reaction.

7- Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

8- Miscellaneous Photochemical Reactions

Photo-Fries reactions of anilides. Photo Fries rearrangement.

Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog.

Photo degradation of polymers, Photochemistry of vision.

Paper-II Spectroscopy (Compulsory for all branches) 60Hrs.

1**- Ultraviolet Visible Spectroscopy**

Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds ultraviolet spectra of aromatic and heterocyclic compounds Steric effect in biphenyls.

2- Infrared Spectroscopy Instrumentation and sample handling.

Characteristic vibrational frequencies of alkanes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, Detailed study of Vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds), Effect of hydrogen bonding and solvent effect on vibrational frequencies.

Symmetry and shapes of AB, A_2, AB_2, AB_3, AB_4, AB_5, and AB_6, mode of bonding of ambidentate ligand, ethylenediamine and diketonato complexes, application of resonance

3**- Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)**

Definition, deduction of absolute configuration, octant rule for ketones.

4**- Nuclear Magnetic Resonance Spectroscopy**

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism, of measurement chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), Intensity of NMR regnals, chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra) virtual coupling, stereochemistry hindered rotation, karlus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transforms technique, Nuclear Overhauser Effect (NOE) Resonance of other nuclei-F, P. Some applications including biochemical systems.

5- Carbon-13 NMR Spectroscopy

General Considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants, Introduction to 2 D NMR.

6- Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as pH_4, F_2- and (BH3).

7- Mossbauer spectrocopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{2+} and Sn^{4+} compounds –nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Book suggested-

1- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.

2- Physical Methods for Chemistry, R.S. Drago, Saunders Company.

3- Structural Methods in Inorganic chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock. ELBS.

4- Infrared and Raman Spectra : Inorganic and Coordination compounds, K. Nakamoto. Wiley.

5- Progress in Inorganic Chemistry vol., 8. ed, F.A. cotton, vol., 15, ed. S.J. Lippard, wiley.

6- Transition Metal Chemistry ed, R.L. Carlin vol. 3 Dekker.

7- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.

8- NMR, NOR, EPR and Mossbauer spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis.

9- Horwood. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeugh and G.J. NBrtin. Heyden.

10- Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus. Wiley.

Paper-III Analytical Chemistry (Compulsory for all branches) 60Hrs.

1- Introduction

Classification of analytical methods-classical and instrumental, types of instrumental analysis, selecting an analytical method.

2- Errors and Evaluation :

Definition of terms of mean and median, precision-standard deviation, relative standard deviation, accuracy, absolute error. Types of error in experimental data-determination (systematic), intermediate (random) and gross. Sources of errors and the effect upon the analytical results methods for reporting analytical data. Statistical evaluation of data indeterminate errors. The use of statistics.

3- Radiochemical methods :

Elementary working, Principles of Geiger Muller, Iionization, proportional and γ -ray counters. Neutron radiation sources, radio tracer techniques. Nautron Activation Analysis (NAA) : Principle, Techniques and applications in preparation of some commonly used radioactive isotopes. Use of radioactive isotopes in analytical and physiochemical problems, Isotopic Dilution Analysis (IDA), substoichiometric IDA, advantages and limitations of IDA and comparison of IDA with NAA. Principle of Radiometric Titrations, Types, Experimental techniques and its applications.

4- Thermal methods of Analysis :

Introduction of different thermal methods, Thermogravimetry- TGA & DTA, static thermogravimetry, quasithermogravimetry and dynamic thermogravimetry, Instrumental and balances, X-Y recorder,

thermogram, factors affecting thermograms. Application of thermogravimetry.

Differential Scanning Calorimetry (DSC) : Introduction, instrumentation, DSC-curves, factors affecting DSC curves and applications.

Thermometric Titrations : Introduction, Instrumentation, apparatus, theory and applications.

5- **Chromatographic Techniques :**

Adsorption and Partition Chromatography, Paper Chromatography, Thin Layer chromatography lon exchange and Gas chromatography, HPLC, Size Exclusion Chromatography, their principles, techniques and important applications.

6- **Electroanalytical Techniques :**

A- **Voltametry :**

General introduction, Principle, Instrumentation, types of Voltammetry Paleography (Principle & Instrumentation), Cyclic Voltammetry, Pulse Methods.

Stripping Technique : Anodic and Cathodic Stripping Voltametry and their applications in the trace determination of metal ions and biologically important compounds.

B. Ion Selective Electrodes :

Electrical Properties of membrane, Glass electrode with special reference to H^+, Na^+, K^+ ions, operation of solid membrane electrode, operation of liquid membrane electrode, coated type ion electode. Applications of ion selective electrode in determination of some toxic metal and some anions (F^-, CI^- Br, I^-, and NO^-_3).

Book suggested :

1. Quantitative Analysis : Day and Underwood.
2. A text book of Quantitative Analysis A.I. Vogal.
3. Advanced Analytical Chemistry : Meites and Thomas
4. Analytical Chemistry : Dr. R.K. Soni
5. Instrumental Methods of Chemical Analysis : G.W. Ewing
6. Physical Methods in Inoganic Chemistry : R.S. Drago
7. Analytical Chemistry : G.D. Christaion
8. Basic Concepts of Analytical Chemistry : S.M. Khopkar
9. Polarography : Kolltarth and Lingane
10. Instrumental Methods of Chemcial Analysis : Braun
11. Instrumental Methods of Analysis : Willard, Merritt & Dean.
12. Analytical Chemistry : Strouts, Crifillan & Wilson.
13. Introduction to radiation Chemistry : J.W.T. Spinks & R.J. Woods.
14. Fundamentals of Analytical Chemistry : S.A. Skoog & D.W. West.
15. Analytical Chemistry : R.V. Dilts
16. EDTA Titration : Flaschka.

Paper-IV Bioinorganic Chemistry Elective 1 60Hrs.

1- Introduction:

Chemistry of amino acids proteins and their derivatives; methods of isolation and identification; Primary, secondary, tertiary and quaternary structures of proteins; determination and biochemical applications of the structures proteins; Nomenclature of nucleosides and nucleotides; Effects of

acid and alkali on hydrolysis of nucleic acids ; Structure of DNA and RNA ; prokaryotic versus eukaryotic organisms.

2- **Metal lons in Biological Systems :** Essential and trace metals.

3- **Na^+/K^+ pump :**Role of metals ions in biological processes.

4- **Bioenergetics and ATP Cycle**

Standard Gibbs energy change in biochemical reactions, exergonic and endergonic. Hydrolysis of ATP, synthesis of ATP and ADP.

DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, photo system I and photo system II in cleavage of water.

5- Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

6- Electron Transfer in Biology

Structure and function of metalloproteins in electron transport process-cytochromes and ion-sulphur proteins, synthetic models.

7- Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Books Suggested:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Book.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.

3. Inroganic Biochemistry vols I and II. ed. G.L. EichhHn, Elservier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard Wiley.
5. Principles of Biochemistry,A.L. Lehninger, Worth Publishers.
6. Biochemistry, L. Stryer, WH. Freeman.
7. Biochemistry, J. David Rawn, Neil Patterson.
8. Biochemistry, Voet and Voet, John Wiley.
9. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
10. Biorganic Chemistry : A chemical Approach to Enzyme Action, H. Duga, and C. Penny.
11. Macromolecules : Structure and Function, F. Wold, Prentice Hall.

Paper-IV Bioorganic Chemistry **Elective 1 60 Hrs.**

1. Introduction:

Chemistry of amino acids proteins and their derivatives; methods of isolation and identification; Primary, secondary, tertiary and quaternary structures of proteins; determination and biochemical applications of the structures proteins; Nomenclature of nucleosides and nucleotides; Effects of acid and alkali on hydrolysis of nucleic acids ; Structure of DNA and RNA ; prokaryotic versus eukaryotic organisms.

2. Enzymes :

Introduction and historical perspective, Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction

and purification. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelismeten and Lineweaver-Burk Plots, reversible and irreversitble inhibition.

3. **Mechanism of Enzyme Action**

   Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, rebonuclease, lysozyme and carboxypeptidase A.

4. **Kinds of Reactions Catalysed by Enzymes**

   Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates, intermediates in isomerization reactions, cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

5. **Co-Enzyme Chemistry**

   Co-Factors as derived from vitamins, co-enzymes, prosthetic groups, apoenzymes. Structure and biological functions of co-enzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B12 Mechanisms of reactions catalyzed by the above co-factors.

6. **Enzyme Models**

   Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers. Cyptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzyme of synzymes.

7. **Biotechnological Applications of Enzymes**

   Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on

enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and chesse-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy.enzymes and recombinant DNA technology. Application of enzymes in organic synthesis.

Books suggested :

1. **Bioorganic Chemistry :** A Chemical Approach of Enzyme Action, Hermann Dugas and Penny, Springer Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. **Enzyme Chemistry :** Impact and Applications, Ed. Collin J Suckling, chapman and Hall./
4. Enzyme Meachanisms Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
5. Fundamentals of Enzymolgoy, N.C. Price and L. Stevens. Oxford University Press.
6. **Immobilized Enzymes :** An Introduction and Applications in Bitechnology, Michael D. Traven, John Wiley.
7. Enzymatic Reaction Mechanisms, C Walash, W-H. Freeman.
8. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
9. **Biochemistry :** The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

Paper-IV Biophysical Chemistry Elective 1 60 Hrs.

1. **Introduction:**

Chemistry of amino acids proteins and their derivatives; methods of isolation and identification; Primary, secondary, tertiary and quaternary structures of proteins; determination and biochemical applications of the structures of proteins; Nomenclature of nucleosides and nucleotides; Effects of acid and alkali on hydrolysis of nucleic acids ; Structure of DNA and RNA ; prokaryotic versus eukaryotic organisms.

2. **Biological Cell and its' Constituents**

Biological cell, Structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

3. **Bioenergetics**

Standard Free energy change in biochemical reactions, exergonic, endergonic Hydrolysis of ATP, synthesis of ATP from ADP.

4. **Statistical Mechani in Biopolymers.**

Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

5. **Biopolymer interactions**

Forces involved in biopolymer interactions. Electrostaic charges, and molecular expansion, hydrophobic forces. Dispersion force interactions. Multiple equlibria and various types of binding processes in biological systems. Hydrogen ion titration curves. DNA Protein Interaction.

6. **Thermodynamics of Biopolymer Solutions**

Thermodynamics of biopolymer soluctions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechnochemical system.

7. Cell Membrane and Transport of Ions

Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

8. Biopolymers and their molecular Weights

Evaluation of size, shape molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion. Sedimentation velocity, viscosity, electrophoresis and rotational motions.

III SEMESTER

ANALYTICAL PRACTICAL

1. To verify Lambert's Beer's Law with the help of U.V. visible spectrophotometer.
    a. To determine max of a given sample.
    b. To determine the concentration of unknown sample with the help of U.V. visible spectrophotometer.
2. To determine the concentration of Na^+, Ca^+, K^+ with the help of flame photometer.
3. To scan the U.V. visible spectra of unknown sample with the U.V-visible double beam spectrophotometer.
4. To determine the calorific value of unknown sample.
5. To determine the degradation peak. Tg, Tm of unknown sample with the help of DSC.
6. To determine kinematic viscosity of plasticizer with the help of Redwood viscometer.
7. To determine the dynamic viscosity of polymeric plastcizer at different temperature with the help of Brook field viscometer.
8. To separate the chlorophyll pigments with the help of TLC.
9. Apply paper chromatography to separate.
    a. The chlorophyll pigments.
    b. Lead anions and cations.
10. To separate the amino acids with the help of TLC.

11. To determine formation constant of Fe SCN^{-2} compounds by conductometry.
12. To determine rate constants & formation constants of intermediate complex in the reaction of Cerium (IV) ammonium nitrate and hypo phosphoric acid in avid medium.

BIOCHEMISTRY PRACTICAL

1. To make a phosphate buffer of pH.
2. Qualitative test for carbohydrates.

   Molish's Iodine, Scliwanhoff, Benediet, Anthrone, Barfoed, Fehling, Bial's Test
3. Qualitati ve test for lipids.

   Acrolien test for presence of FA, Test for unsaturation of FA.
4. Determination of acid value of fats and oils.
5. Determination of saponification value of fats and oils.
6. Determination of Iodine no. of a fat sample.
7. Qualitative test for Amino acid and protein.

   Ninhydrin, Million's, Sakaguchi, Xanthoproteic, Biuret.
8. To detect Ketone bodies in urine sample.
9. Separation of plant pigmen by TLC.
10. Estimation of amylase activity in saliva.
11. To Know blood group in given sample of blood.
12. To have RBC and WBC count.
13. To estimate glucose in urine sample.
14. To estimate sugar in blood.
15. To prepare casein protein from milk and its estimation.