

JAWAHARLALNEHRUTECHNOLOGICALUNIVERSITY GURAJADA

VIZIANAGARAM

Course Structure and Syllabus for Pre-Ph.D

CHEMISTRY

PART-I

S.NO	PAPER	PAPERCODE
1	AdvancedInstrumentalMethodsfor ChemicalCharacterizationandAnalysis	PH24BC101
2	AnalyticalChemistry	PH24BC102
3	OrganicChemistry	PH24BC103

PART-II

S.NO	PAPER	PAPERCODE
1.	Inorganic Chemistry	PH24BC201
2.	Physical Chemistry	PH24BC202
3.	Chemistry & Environment	PH24BC203
4.	Chemistry of Biological Processes	PH24BC204
5.	Advanced Topics in Chemistry	PH24BC205
6.	Chemistry of biologically active compounds	PH24BC206
7.	Chemistry of Life	PH24BC207
8.	Supra molecular Chemistry	PH24BC208
9.	Chemistry of Energy Systems	PH24BC209
10.	Chemistry of Polymers and their Applications	PH24BC210

**(PH24BC101) ADVANCED INSTRUMENTAL METHODS FOR CHEMICAL
CHARACTERIZATION AND ANALYSIS**

Unit-1: UV-Visible and IR Spectroscopy:

Introduction; Absorption Laws; Theory of Electronic Spectroscopy; Types of Electronic Transitions; Chromophore concept; Auxochrome; Solvent effect; Instrumentation; Woodward – Fischer rules for calculating absorption maxima in dienes and α,β -unsaturated carbonyl compounds; Steric hindrances and co-planarity; Estimation of ligand-metal ratio in complexes; Applications.

Introduction of IR; basic principles of IR; Selection rules, Normal modes of vibrations, finger print region, group frequency region, Instrumentation, Qualitative, Quantitative analysis and Applications.

Unit-2: Atomic Absorption and Emission Spectroscopy

Absorption Spectroscopy Introduction and importance; principles and instrumentation; Interferences - Chemical & Spectral Evaluation methods; Applications for qualitative and quantitative analysis.

Emission Spectroscopy: Flame photometry; emission spectroscopy and ICP-OES-Principles and instrumentation; Evaluation methods and applications, Fluorescence and Phosphorescence methods.

UNIT-3. Chromatographic Techniques:

Gas Chromatography; HPLC, LC-MS & GC-MS: Introduction, basic principle and instrumentation, Comparison of GC and HPLC; Qualitative analysis, Quantitative analysis and Applications

Unit-4: Nuclear Magnetic Resonance and Mass Spectroscopy

Nuclear magnetic resonance Spectroscopy: Principles of NMR, High resolution NMR – chemical shift, factors affecting the chemical shift, Spin-Spin coupling, Spin-Spin and Spin-lattice relaxation, decoupling, Chemical exchange, structure determination, hydrogen bonding; geometrical isomerism and applications of proton NMR, ^{13}C -NMR spectroscopy principles and advantages.

Mass Spectroscopy: Introduction; basic principles, Instrumentation: ionizing sources, types of ions and applications.

Unit-5: Polarography & Cyclic voltammetry:

Polarography: Principles-Polarographic wave, diffusion current, Half wave potential; effect of complex formation on diffusion current, polarographic maxima, qualitative analysis and, Quantitative analysis, Inorganic and Organic applications.

Amperometry: Principles, amperometric titrations

Cyclic Voltammetry: Reversible and irreversible process; evaluation of number of electrons in a chemical reaction, application to Diphenyl fulvene.

References:

1. “Vogel’s Text Book of Quantitative Chemical Analysis”, by J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, Pearson Education Pvt. Ltd., New Delhi, (6th edition).
2. “Analytical Chemistry – Problems & Solutions”, by S.M.Khopkar, New Age International Pvt. Ltd., New Delhi, (2002).
3. “Applications of Absorption Spectroscopy of Organic Compounds” by John R.Dyer, Prentice-Hall of India Pvt. Ltd., New Delhi (1969).
4. Instrumental Methods of Analysis by Hobart H. Willard and D.U. Merritt & J.R.J.A. Dean, C.E.S Publishers and distributors.
5. Instrumental methods of chemical analysis – By Scoog and West, Broadway Publishers.
6. Physical chemistry and Inorganic chemistry – By R.S.Drago, East Press New Delhi.
7. Electro organic studies By A.J.Fry (Page No. 93-95) Harper and Row, New York:1972.

(PH24BC102) ANALYTICAL CHEMISTRY

Unit: 1 Treatment of analytical data:

Precision and accuracy, relative accuracy, standard deviation, coefficient of variation, confidence interval, Types of errors-- Sources of determinate errors and their elimination, random errors and their distribution, propagation of determinate errors and random errors, Control charts, Statistical tools – „F“ test, „t“ test and „Q“ test; Method of least squares; Correlation coefficient and coefficient of determination; Limit of detection(LOQ) ; Limit of determination(LOD) Sensitivity and selectivity of an analytical method, Analysis of variance (ANOVA).

Unit:2 Solvent Extraction:

Factors favouring solvent extraction, Distribution constant and Distribution Ratios; Method of extraction, treatment of extraction; Counter current Liquid-Liquid Extraction; Continuous Liquid-Liquid counter current extraction; Application of solvent extraction, Quantitative treatment of solvent extraction - Extraction reagents. Concept of synergistic extraction. Applications:- (i). Determination of ferric ion as chloride.(ii).Determination of nickel by synergistic extraction using dithiozone and 1,10-phenanthroline. (iii). Determination of Molybdenum by thiocyanate method.

Unit:3 Oxidation and Reduction equilibria and Complexometric titrations:

Oxidation and Reduction equilibria : Galvanic Cell, Nernst Equation, Types of Electrodes, Equilibrium constants from standard Potentials, Formal potentials and other approximations, Titration curves, Feasibility of Redox titrations, Redox indicators and their structural chemistry, Reagents used for Preliminary Redox reactions, Reducing agents, Potentiometric methods of analysis, indicator Electrodes –Potentiometric titration.

Complexometric titrations: Stability of complexes, Chelate effect and Metal ion indicators
Titrations involving multi-dentate ligands

Unit:4 Thermal Analysis:

Principles, basic instrumentation and applications of Thermal Gravimetric Analysis (TGA), Differential Thermal Analysis (TG-DTA) and Differential Scanning Calorimetry (DSC), Temperature Programmed reduction/Oxidation/ desorption/sulphidation, thermal conductivity and thermal diffusivity.

Unit:5 X-ray Methods of analysis:

XRD: X-ray diffraction; Principles, Braggs law, Basics of Crystallography, Derivation of percentage crystallinity and crystallite size, Debye-Scherrer Equation, Application of XRD and Phase Identification.

XRF: Principles, Instrumentation, types of XRF applications and limitation.

XPS: Principles, Instrumentation, applications and limitation.

References:

1. Quantitative Analysis by Day & Underwood, Erinoice silver of India Pvt. Ltd.
2. Fundamentals of Analytical Chemistry by SKoog & West
3. Instrumental Methods of Analysis by Hobart H.Willard and D.U.Merritt & J.R.J.A.Dean, C.E.S Publishers and distributors.
4. Text book of Quantitative Inorganic Analysis by A.I.Vogel, Pearson Publisher.
5. Separation methods- by M.N.Sastry
6. Chemical methods of separation by John.O.Dean, CBS Publishers & Distributors, New Delhi.
7. Physical Chemistry by Gardon and M. Barrow.
8. Analytical Chemistry by Dilts



(PH24BC103) ORGANIC CHEMISTRY

UNIT-1: Stereochemistry:

Optical Isomerism - Elements of symmetry and chirality – Configuration of optically active molecules, dl and RS notations - Relative and Absolute configurations- Resolution of Racemic mixtures. Cram's rule - Concept of dynamic enantiomerism, CD and ORD methods. Geometrical Isomerism: Determination of E-Z configuration by chemical and spectral methods.

UNIT-2: Role of organic reaction intermediates and mechanism:

Organic reaction intermediates: Classical and Non-Classical carbocations, Structure, stability, shape Reactivity of Carbonium ions; Carbanions; use of Carbanions in synthesis; Free radicals; carbenes; nitrenes and benzyne.

Organic Reaction Mechanisms: Kinetic and non-kinetic methods; Uses of isotopes; Cross-over experiments; Intermediate trapping. Kinetic versus Thermodynamic control, Linear free energy – relationships.

Unit-3: Aromatic Substitution reactions:

Electrophilic: Electrophilic aromatic substitution in activated benzene derivatives; Reimer – Tiemann reaction; Vilsmeier – Haack formylation; Houben – Hoesch reaction; Diazo – Coupling; Hofmann – Martius rearrangement.

Nucleophilic: Aryl halides; Low reactivity of aryl and vinyl halides; SN^1 , SN^2 and benzyne mechanisms; Reactivity and Orientation in nucleophilic aromatic substitution; Nucleophilic substitution – aliphatic and aromatic; Von – Richter rearrangement and Sommelet – Hauser rearrangement.

Unit-4: Addition to Carbon – Hetero atom multiple bonds:

Addition reactions of Carbonyl compounds like aldehydes and ketones; Addition of Oxygen nucleophiles like water, alcohols, glycol, Addition of Carbon nucleophiles like cyanide and carbanion, Addition of Sulphur nucleophiles like thiols and $NaHSO_3$. Addition of nitrogen nucleophiles like ammonia, amine, phenyl hydrazine, 2,4-dinitrophenyl hydrazine, Addition of hydride ion – Reduction of aldehydes and ketones with $NaBH_4$ and $LiAlH_4$.

Unit-5: Condensation reactions of Carbonyl compounds:

Aldol condensation; Canizzaro reaction; Dieckmann condensation; Benzoin condensation; Reformatsky reaction; Knoevenegal condensation; Addition of Grignard reagents to aldehydes and ketones.

References:

- 1) “*Stereochemistry of Carbon Compounds*” by Ernest L.Eliel, Tata-Mc Graw Hill Co., New Delhi (1975).
- 2) “*Stereochemistry- Conformation and Mechanism*”, by P.S. Kalsi, Wiley Eastern Ltd., New Delhi, Hyd. (1991).
- 3) “*Advanced Organic Chemistry*”, by Jerry March, John Wiley & Sons, New York, London. (2001).
- 4) “*Organic Chemistry*”, by R.T.Morison and R.N.Boyd, Allyn & Bacon Inc., (printed in Singapore) (2001).
- 5) “*Organic Chemistry*”, by Paula Yurkanis Bruice, Pearson Education (Singapore) Pvt. Ltd., Delhi (2001).
- 6) “*A Guide-book to Mechanism in Organic Chemistry*”, by Peter Sykes Orient Longmans Ltd., New Delhi (1976).
- 7) “*Mechanism and Theory in Organic Chemistry*”, by T.H.Lowry and K.S. Richardson, Harper & Row Publishers, London (1988).

(PH24BC201) INORGANIC CHEMISTRY

UNIT- 1 : Symmetry and group theory in chemistry

Symmetry elements and symmetry operations; Point groups: Mathematical requirements for a point group; Schoenflies notations point groups; Systematic assignment of molecules to point groups; Sub-groups; Classes; Matrix representation of symmetry elements; Matrix representation of C_{2v} , C_{3v} and C_{4v} point groups; Reducible and Irreducible Representations; Properties of Irreducible representations; Construction of character tables (C_{2v} and C_{3v} point groups); Mulliken symbolism rules for IRs; The standard reduction formula; The Direct product; Symmetry criteria for Optical activity; Symmetry restrictions on Dipole moments; Symmetry and Stereo-isomerism; Prediction of IR and Raman spectral activity of H_2O molecule.

UNIT- 2: Coordination chemistry

Werner's theory Representative ligands, Nomenclature; Constitution and geometry- Coordination number, polymetallic complexes; Isomerism and Chirality- Square planar, Tetrahedral and octahedral complexes, ligand chirality

Metal ligand Bonding: Crystal Field Theory (CFT) for bonding in transition metal complexes, crystal field splitting of d - orbitals in octahedral, tetrahedral, tetragonal and square planar fields. Crystal Field Stabilization energy (CFSE) and its calculation in six and four coordinated complexes, Spectrochemical series with reference to ligands and metal ions. Factors affecting the magnitude of Δ_o in octahedral complexes, Jahn-Teller effect and its consequences

Thermodynamic origin- Step-wise and overall stability of the complex, Chelate, macrocyclic and cryptate effects; Determination of stability constant of a complex using pH metry, spectrophotometry and polarographic techniques. Magneto Chemistry: diamagnetism paramagnetism, ferro-and anti-ferromagnetism, susceptibility, magnetic moment, super exchange, Curie-Weiss law.

UNIT- 3: Electronic spectroscopy of transition metal complexes

Energy levels in an atom, microstates – calculation of microstates; Spectroscopic states – coupling of orbital angular momenta and spin angular momenta; Spin – orbit coupling (R-S coupling) Derivation of term symbols for p^2 and d^2 configurations. Determination of ground state terms – Hund's Rules; Hole formalism. Electronic spectra of octahedral and tetrahedral complexes. Nature of electronic spectrum; Laporte orbital and spin selection rules; Transforming spectroscopic terms into Mulliken symbols. Spectra of d^1 to d^9 metal ions/complexes. Orgel diagrams, Tanabe Sugano diagrams and comparison between these diagrams. Charge transfer ($L \rightarrow M$ and $M \rightarrow L$) spectra in inorganic compounds. Nature of electronic spectra of f-block metal complexes.

UNIT- 4: Organometallic chemistry

Classification of ligands based on hapticity and polarity; σ and π – bonded organometallics; 18 electron rule, General methods for the preparation of main group and Transition metal organometallics.

Types of organometallic reactions, oxidative additions, reductive eliminations, insertion.

Nature of M-C bond Synthesis, bonding and uses of organometallic compounds – Two electron ligands (olefinic and acetylenic complexes) Three electron ligands (Allylic complexes), Four electron ligand (Butadiene and Cyclobutadiene complexes) Five electron ligand (Ferrocene complexes)

UNIT- 5: Metal complexes in catalysis and medicine

Homogeneous and Heterogeneous catalysis - Olefin hydrogenation, dimerization and isomerization - Hydroformylation - water gas shift reaction – Effects of surface site on adsorption - The Fischer – Tropsch Process; Ziegler – Natta olefin polymerization - Ammonia synthesis

Metal complexes in Medicine: Metal deficiency and diseases; Toxic effects of metals; Metals used for diagnosis and chemo therapy. Gold complexes in the treatment of Rheumatoid arthritis; Anti-cancer Drugs platinum ammine halide; Metallocenes and gold complexes; platinum anticancer drugs – A case study of Bioinorganic chemistry of platinum anticancer Drugs; Design of new Inorganic anticancer Drugs; Determination of antibacterial and anti-fungicidal activities of metal complexes.

Suggested Books

1. Concise Inorganic chemistry by J.D. Lee ELBS 4th Edition, 1994.
2. Inorganic Chemistry by Shriver and Atkins Oxford University press 4th Edition, 1999.
3. Structural methods in Inorganic chemistry. E.A.V Ebsworth, David W.H. Rankin and S.Cradock (Great Britain) ELBS, 1987.
4. Bertini, H.B. Gray, S.J. Lippard and J.S Valentine Bioinorganic Chemistry, Viva books pvt., Ltd., New Delhi, 1998.
5. Organometallic Chemistry – A Unified Approach by R. C. Mehrotra and A. Singh.



(PH24BC202) PHYSICAL CHEMISTRY

Unit-1: Photochemistry:

Types of Photochemical reactions; Laws of Absorption (Grothuss-Draper law & Einstein's law); Quantum yield; Primary & Secondary Photochemical processes; Jablonski Diagram: Fluorescence, Phosphorescence, Inter-System Crossing; Internal Conversion-Vibrational Cascade and Chemiluminescence.

Kinetics of Photochemical reactions; Dissociation of HI; Reaction between Hydrogen and Chlorine.

Unit-2: Catalysis and Enzyme Catalysis:

Catalysis : Types of Catalytic Reagents; Types of Catalysis (Homogeneous and Heterogeneous catalysis); Catalytic activity; Acidity Functions; Acid-Base catalysis, Theory of Homogeneous catalysis; Theory of Heterogeneous catalysis (Chemical theory & Adsorption theory); Kinetics of heterogeneous reactions.

Enzyme Catalysis : Specificity in Enzyme Catalyzed reactions; Michaelis- Menten mechanism; Influence of Concentration on Enzyme-Catalyzed reactions; Influence of Temperature on Enzyme Catalyzed reactions.

UNIT-3: Quantum Mechanics

Introduction to Quantum Mechanics: Postulates of Quantum Mechanics; Schrödinger equation; Physical significance of wave function; Eigen values and Eigen functions; Particle in a one dimensional box; Normalization; Orthogonality; Degeneracy.

Variation method & Perturbation theory; Applications to the Helium atom; Anti -symmetry and exclusion principle; Slater's determinantal wave functions.

Unit-4: Phase rule and Surface Chemistry:

Phase rule : Definition of Phase rule; Terminology in Phase rule; Phase diagram of two & three component systems; Stokes and Roozboom representation for three component systems-applications

Surface Chemistry : Adsorption; Factors influencing adsorption; Surface area and its measurements; Adsorption isotherm curves; Langmuir's adsorption isotherm- its limitations; B.E.T. Adsorption isotherm-its applications; Negative adsorption; Positive adsorption; Chemisorption; Physisorption and Determination of surface area.

Unit-5: Chemical Kinetics and Thermodynamics:

Ionic reactions: Influence of solvent on the rate of reactions (single & double sphere A.C. model); Primary salt effect; Secondary salt effect; Influence of frequency factor; Influence of ionic strength.

Chain Reactions: Steady state treatment, $\text{H}_2\text{-Br}_2$ & $\text{H}_2\text{-O}_2$ reactions, Explosion limits

Thermodynamics: Laws of thermodynamics, Enthalpy and chemical reactions, isothermal and adiabatic processes, Carnot cycle, Entropy and spontaneous process, free energy, Gibbs and Helmholtz energies, standard Gibbs free energy of reaction, applications of thermodynamics.

Dilute solutions: Raoult's law, Henry's law, Boiling point elevation, Freezing point depression.

References:

1. ***“Physical Chemistry”*** by Samuel Glasstone and D. Lewis; Mc Millan India Ltd. New Delhi (2nd Edition, 1984).
3. ***“Physical Chemistry”*** by Peter Atkins and J.D.Paula; ELBS, Low Price Edition (7th, Edition, 2002).
4. ***“Chemical Kinetics”*** by K.J.Laidler; Tata Mc Graw- Hill Publishing Company Ltd, New Delhi (2nd Edition, 1984).
5. ***“Principles of Physical Chemistry”*** by Maron and Prutton; Oxford and IBH Publishing Co Pvt Ltd (New Delhi) and Calcutta (4th Edition, 1966).
6. ***“Physical Chemistry through problems”*** by S.K.Dogra and S.Dogra; New Age International Pvt Ltd, New Delhi and Hyderabad (4th Edition, 1996).
7. ***“Chemical Kinetics and Catalysis”*** by G.M. Panchenkov and V.P.Lebedev. ***“Foundation of Chemical Kinetics”*** by E.N. Yereimin.
8. ***“Physical Chemistry”*** by Peter Atkins and J.D.Paula, 2nd Edition, Mc Millan India Ltd. New Delhi (1984).
9. ***“Quantum Chemistry”*** by A.K.Chandra, 3rd edition, Tata Mc Graw-Hill Publishing Pvt Ltd., New Delhi (1988).
10. ***“Quantum Chemistry”*** by R.K.Prasad, 3rd edition, New Age International Publications (1997).
11. ***“Quantum Chemistry”*** by I.N. Levine, 4th edition, Prentice Hall of India Pvt Ltd (1994).

(PH24BC203) CHEMISTRY & ENVIROMENT

Unit-1: Chemistry of Air Pollution:

Introduction: environmental pollution; Concepts, nomenclature and segments; Composition of atmosphere; Pollution of atmosphere; Types of air pollutants; Primary and Secondary air pollutants; Effect of air pollutants on health and environment- Oxides of Carbon, Sulphur, Nitrogen, Ammonia and Hydrocarbons, Ozone, Chloro-fluoro carbons, gasoline and lead.

Reducing toxic emission from the fuel combustion in vehicles; Control of NO_x and Lead emission; Catalytic control device for automobiles. Greenhouse effect, Acid rain, Photochemical smog and Elnino Phenomenon.

Unit-2: Chemistry of Water Pollution:

Environmental role of water; Hydrological cycle of water; Classification of water pollutants; Measurement of BOD, COD, TOC, Salinity and dissolved oxygen; Effect of waste chemicals; oil spills and heavy metals; waste water treatment - Primary, Secondary (Aerobic & Anaerobic) and Tertiary treatment.

Unit-3: Chemistry of Soil Pollution and Agricultural Waste:

Soil pollution: Definition, causes. Effects: Health and Ecosystem, Classification of Soil Pollutants; Source and Classification and their effects.

Agricultural Waste:

Pesticide: Classification of Pesticides; Environmental implication of Pesticides; Alternate methods of Pest Control; Control methods of Pesticide Pollution

Chemical Fertilizers: Classification, effects and remedies.

Unit-4: Thermal, Radioactive and Noise pollution:

Thermal Pollution: Sources, Causes, Effects and Remedies.

Radioactive pollution : Sources, Control measures, Disposable methods, Chernobyl Nuclear accident.

Noise pollution : Sources, Causes, types effects and control measures,.

Unit-5: Pollutants from Industry and Solid waste management

Pollutants from Industry: Polymers and Plastics; Sugar and Distillery; Drugs and Pharmaceuticals; Paper and Pulp; Metallurgical industries; Minimata disasters, Bhopal gas disaster.

Solid waste management: Types of solid waste, sources, effects of solid waste, industrial solid waste management, disposal, methods of solid waste managements and recycling.

References:

1. ***“Environmental Chemistry”***, by V.P. Kudesia, Pragathi Prakashan, Meerut, **(2003)**.
2. ***“Fundamental Concepts of Environmental Chemistry”***, by G.S. Sodhi, Narosa Publishing House Pvt. Ltd., New Delhi, **(2002)**.
3. ***“A Text Book in Environmental Science”***, by V. Subramanian, Narosa Publishing House Pvt. Ltd., New Delhi, **(2002)**.
4. ***“Environmental Chemistry”***, by A.K. De, New Age International Publishers, New Delhi, **(2003)**.
5. ***“Solid waste management***, by B.K. Sharma and H. Kaur, Goel Publishing House, Meerut,**(1999)**.
6. **Environmental chemistry** by Manahan, CRC Press.
7. **Environmental chemistry** by Moore & Moore, Amazon.
8. **Solid waste treatment** by Manhan, Natural environment agency.



(PH24BC204) CHEMISTRY OF BIOLOGICAL PROCESSES

UNIT-1: Cell Chemistry:

Introduction to cell as the basic unit of Life; Types of cells; Procaryotes and Eucaryotes – examples; Characteristics of Plant & Animal cells; Structure of Cell and its organelles and their functions;

A Chemical probe into the Cell: Cell Wall composition - (G+) & (G-) Procaryotes, Plant and Animal cells i) Minerals, ii) Carbohydrates, iii) Proteins, iv) Lipids, v) Nucleic acids, vi) Enzymes, vii) Vitamins, viii) Hormones, their biological functions.

UNIT -2: BIOANALYTICAL CHEMISTRY

Clinical analysis: Collection, Preservation and composition of blood sample, .Clinical analysis of blood glucose, blood urea nitrogen and immunoassay. The blood gas analyzer, Determination of trace elements (Fe, Cu, Zn) in blood sample.

Drug analysis : Classification and nomenclature of natural drugs; biological and chemical classification of drugs, Analysis of drugs using TLC, GC, and HPLC. Spectrophotometric methods for the analysis of drugs. Determination of the concentration of ethyl alcohol in pharmaceutical preparation and alcoholic beverages.

Antibiotics and sulpha drugs: Classification of antibiotics based on chemical structures; Synthesis, Structure, properties, and assay of some antibiotics: 1) Chloramphenacol, (2) Penicillin, 3) Streptomycin, (4) Cibazole.

UNIT -3: BIOINORGANIC CHEMISTRY

(a) Essential and Trace Elements: Concept of essentiality, role of metal ions in biological processes, Na^+/K^+ Pump.

(b) Photosynthesis: Structure of Chlorophyll, Photosynthetic mechanism in bacteria and in green plants [Z-Scheme (PS-I & PS-II)], Role of manganese complex in the cleavage of water, Model systems.

(c) Respiration (Transport and storage of dioxygen): Structure and functions of myoglobin, hemoglobin, Hemerythrin and hemocyanin, model systems.

(d) Biological nitrogen Fixation: Molybdenum nitrogenase, Mechanisms of biological N_2 fixation, model systems.

UNIT -4: BIOORGANIC CHEMISTRY (BIOMOLECULES)

(a) **Nucleic acids:** Introduction. Isolation of nucleic acids. Hydrolysis products of nucleic acids. Structure of heterocyclic bases - Adenine, Guanine, Cytosine, Thymine and Uracil. Structure of sugars – Ribose and 2-deoxyribose. Primary, secondary and tertiary structures of DNA, Types of RNA - mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis.

(b) **Enzymes :** Introduction. Definition. Composition. Nomenclature and Classification based on mode of action. Mechanism of enzyme activity, Factors affecting enzyme catalysis. Lock and Key model and Induced-Fit model, Enzyme inhibition– Irreversible inhibition, Competitive inhibition and Non-competitive inhibition, Immobilized enzymes.

UNIT -5: BIOPHYSICAL CHEMISTRY (Bio Membranes & Bioenergetics)

(a) **Biological membranes:** Chemical composition of cell membranes; Membrane Models; Functions of cell membrane; Mechanism of ATP Synthesis

(b) **Bioenergetics :** Importance of Bioenergetics; Energy and its Various forms; Principles of Thermodynamics; Entropy; Free Energy; Relation between ΔG and ΔS ; Relationship between Standard Free Energy Change and Equilibrium Constant; Bio-chemist's standard state; Standard Free Energy changes at pH 7 of $\Delta G^{\circ'}$; Difference between ΔG and $\Delta G^{\circ'}$; Standard free energy values of Chemical reactions.

Recommended Books

1. Standard methods of Chemical analysis by Welcher.
2. Inorganic Chemistry by J. E. Huheey, E.A. Keiter and R.A. Keiter, 4th edition, Addison Wesley Publishing Company, New York, 2000.
3. Bioinorganic Chemistry, R.W. Hay, Ellis Horwood Ltd., Chichester, New York. 1984.
4. Bioinorganic Chemistry, K. Hussain Reddy, New Age International Publishers, New Delhi, 2003.
5. Organic Chemistry Vol. 2 Stereochemistry and the Chemistry of Natural Products 5th Edition by I. L. Finar.
6. CHEMISTRY – General, Organic, Biological by Jacqueline I. Kroschwitz and Melvin Winokur.
7. Bio Chemistry by Pawar Chatwal.
8. Bio Physical Chemistry by M.Satake, Y. Hayashi, M.S. Sethi & S.A. Iqbal

(PH24BC205) ADVANCED TOPICS IN CHEMISTRY

Unit.1: Chemistry of Nanomaterials

Introduction: Scope of nanoscience and nanotechnology, nanoscience in nature, classification of nanostructured materials, importance of nano materials.

Synthetic Methods: Bottom-Up approach:- Sol-gel synthesis, microemulsions or reverse micelles, co-precipitation method, solvothermal synthesis, hydrothermal synthesis, microwave heating and sonochemical synthesis.

Top-Down approach:- Inert gas condensation, arc discharge method, aerosol synthesis, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, and chemical vapour deposition method, electrodeposition method, high energy ball milling.

UNIT-2: Studies of Nano-structured Materials and Techniques of Characterization:

Studies of Nano-structured Materials: Synthesis, properties and applications of the following nanomaterials: fullerenes, carbon nanotubes, core-shell nanoparticles, nanoshells, self-assembled monolayers, monolayer protected metal nanoparticles, nanocrystalline materials, magnetic nanoparticles and important properties in relation to nanomagnetic materials, thermoelectric materials.

Techniques for characterization: Diffraction technique, spectroscopy techniques, electron microscopy techniques for the characterization of nanomaterials, BET method for surface area analysis, dynamic light scattering for particle size determination.

UNIT .3: Green chemistry: principles, concepts and environmentally benign solvents

Green chemistry: principles, concepts, Introduction, Green chemistry Principles, sustainable development and green chemistry, atom economy, atom economic reactions: Rearrangement, addition reactions and un-economic reactions: Substitution, elimination and Wittig reactions, Reducing Toxicity. Waste-problems and Prevention: Design for degradation, Polymer recycling.

Environmentally benign solvents: Organic solvents and volatile organic compounds, solvent free systems, supercritical fluids: Super critical carbon dioxide, super critical water and water as a reaction solvent.

UNIT.4: Catalysis and Green chemistry

Introduction to catalysis, Heterogeneous catalysts: Basics of Heterogeneous Catalysis, Zeolites and the Bulk Chemical Industry, Heterogeneous Catalysis in Fine Chemical and Pharmaceutical Industries, Catalytic Converters, Homogeneous catalysis: Transition Metal Catalysts with Phosphine Ligands, Greener Lewis Acids, Asymmetric Catalysis, Heterogenising the Homogeneous catalysts, Phase transfer catalysis: C–C Bond Formation, Oxidation Using Hydrogen Peroxide, Bio-catalysis and photo-catalysis with examples.

UNIT 5: Emerging greener technologies and alternative energy sources

Biomass as renewable resource, Energy: Fossil Fuels, Energy from Biomass, Solar Power, Other Forms of Renewable Energy, Fuel Cells, Chemicals from Renewable feedstocks:

Chemicals from Renewable Feedstocks: Chemicals from Fatty Acids, Polymers from Renewable Resources, Some Other Chemicals from Natural Resources, Design for energy efficiency: Photochemical Processes, Examples of Photochemical Reactions, Electrochemical Synthesis: Examples of Electrochemical Synthesis.

TEXT BOOKS:

1. NANO: The Essentials: T Pradeep, MaGraw-Hill, 2007.
2. Textbook of Nanoscience and nanotechnology: B S Murty, P Shankar, Baldev Rai, BB Rath and James Murday, Univ. Press, 2012.
3. M. Lancaster, Green Chemistry an introductory text, Royal Society of Chemistry, 2002.
4. Paul T. Anastas and John C. Warner, Green Chemistry Theory and Practice, 4th Edition,
Oxford University Press, USA

REFERENCE BOOKS:

1. Concepts of Nanochemistry; Ludovico Cademrtiri and Geoffrey A. Ozin & Geoffrey A. Ozin, Wiley-VCH, 2011.
2. Nanostructures & Nanomaterials; Synthesis, Properties & Applications: Guozhong Cao, Imperial College Press, 2007.
3. Nanomaterials Chemistry, C. N. R. Rao, Achim Muller, K.Cheetham, Wiley-VCH, 2007.
4. Green Chemistry for Environmental Sustainability, First Edition, Sanjay K. Sharma and Ackmez Mudhoo, CRC Press, 2010.
5. Edited by Alvis Perosa and Maurizio Selva , Hand Book of Green chemistry Volume 8:
Green Nanoscience, wiley-VCH, 2013.

(PH24BC206) CHEMISTRY OF BIOLOGICALLY ACTIVE COMPOUNDS

UNIT – 1: Heterocyclic Compounds:

Synthesis, reactivity, properties and importance of furan, thiophene, pyrrole, pyridine, piperidine, quinoline, isoquinoline, and Indole, Benzofuran, Benzothiophene, Coumarin, Chromene, Carbazole and Acridine. Pyrazole, Oxazole, Thiazole, Pyridazine, Pyrimidine and Pyrazine.

UNIT – 2: Molecular Rearrangements:

Nucleophilic, electrophilic and free radical rearrangements – Wagner – Meerwein, Pinacol, Benzil-benzilic acid, Favorski, Fries, Nebe, Hofmann Curtius, Beckmann, Schmidt, Baeyer–Villiger. Perkin, Stobbe, Dieckmann condensations, Knoevenagel condensation, Wittig reaction, Claisen condensation, Mannich reaction, Michael condensation, Robinson annulation, Reformatsky reaction.

UNIT –3: Alkaloids

Alkaloids-source and classification, extraction and general methods for determining structure, Structure elucidation of papaverine, morphine and codeine.

Unit:4 : Terpenoids

Classification, isoprene rule, special isoprene rule and structural elucidation of Santonin and Abietic acids, biogenesis of mono, di and sesqui terpenoids.

Unit 5: Steroids and Prostaglandin

Steroids: Structural determination of Cholesterol, Estrogen and testosterone, biogenesis of cholesterol.

Prostaglandin: Nomenclature, biological effects, biosynthesis, synthesis of prostaglandin, structural elucidation of PGE-1 and E-2 only.

References:

1. Advanced organic chemistry by reaction mechanism and structure (McGraw Hill and Kogakush) by Jerry March.
2. Molecular reactions and photochemistry (Prentice Hall) by Charles Dupey and O.Chapman.
4. Organic Chemistry, 5th edition (Prentice Hall of India) by R.T.Morrison and R.N.Boyd.
5. Organic chemistry vol. I & II(ELBS Longmann group Ltd., London) by I.L.Finar.

6. Organic chemistry, 5th edition, (John Wiley and Sons, New York, 1992) by T.W.Graham Solomons.
7. Organic polymer chemistry by K.J.Samders, Whapman and Hall.
8. Organic chemistry of synthetic high polymers by R.W.Lenz, Interscience Publishers.
New York Principles of Polymerization by G.Odion. John-Wiley, New York.

(PH24BC207) CHEMISTRY OF LIFE

Unit-1: Cell Chemistry:

Introduction to cell as the basic unit of Life; Types of cells; Procaryotes and Eucaryotes – examples; Characteristics of Plant & Animal cells; Structure of Cell and its Organelles and their functions;

A Chemical probe into the Cell: - Cell wall composition - (G+) & (G-) Procaryotes, Plant and Animal cells i) Minerals, ii) Carbohydrates, iii) Proteins, iv) Lipids, v) Nucleic acids, vi) Enzymes, vii) Vitamins, viii) Hormones and their biological functions.

Unit-2: Lipids and Membranes:

Introduction: Lipid Structure - Acyl glycerol, Phospho glycerides (Phospholipids), ether lipids and sphingolipids. Bio-synthesis of lipids. Biological membranes – their role, structural complexity and compositions; Plasma membrane, Membrane lipids, Membrane proteins; Lipid bilayers, Fluid Mosaic Model of biological membrane. Dynamic nature of lipid bilayers and membrane. Protein and Glycoprotein components of membrane. Membrane transport pores and channels, active transport and passive transport.

Unit-3: Enzymatic Processes:

Definition, classification and nomenclature; Factors affecting the enzyme catalysed reactions. Advantages and limitations of enzymes in organic synthesis – mechanistic aspects of enzyme catalysis – Lock and Key mechanism, Induced – Fit mechanism, Desolvation and Solvation – substitution theory, Three- point attachment rule. Factors affecting the enzyme catalysed reactions. Enzyme selectivity – chemo, regio, diastereo and enatio selectivity – illustration with suitable examples. Regulation of enzyme activity – Allosteric enzymes. Enzyme inhibition – reversible inhibition – competitive, non-competitive and uncompetitive inhibition of enzymes. Immobilised enzymes – immobilization by physical and chemical methods. Co-enzymes involved in Oxidation-Reduction processes. Role of metal ions in biological processes, physiology of digestion.

Unit-4: Bio-chemistry of Carbohydrates, Respiration and Carbohydrate Metabolism:

Bio-chemistry of Carbohydrates: Classification of Carbohydrates; Stereoisomerism; Optical isomerism; Optical activity projection and perspective formulae; D-glyceride as a reference compound; Cyanohydrin synthesis; Structure of glucose; monosaccharides, disaccharides and polysaccharides; Polysaccharides and Glycoproteins in cells.

Respiration and Carbohydrate Metabolism: Glycolysis and Krebs's Cycle; Physiology of respiration in mammals, respiratory exchange and transport of respiration at cellular level. Interconversion of glycogen and glucose in liver and the role of insulin.

Unit-5: Chemistry and Bio-chemistry of Amino Acids & Proteins:

General properties of Amino acids; Proteins - Classification and Function; Structure of Proteins – Primary, Secondary, Tertiary and Quaternary Structure of Proteins. Synthesis of Peptides and Poly Peptides. Determination of Structure of Poly Peptides -N-terminal and C-terminal residue analysis.

Bio-chemistry of Nucleic Acids: Introduction; Hydrolysis of Nucleic acids; Structure, Physical and Chemical properties of Heterocyclic bases - Adenine, Guanine, Uracil and Thymine; Structure of DNA: Primary, Secondary, Tertiary structures of DNA. A,B,C and Z forms of DNA. Structure of RNA – types of RNA – mRNA, rRNA and tRNA.; Definition and explanation of Replication, Transcription, Translation. Genetic Code – Codons – Protein synthesis.

References:

1. “*Outlines of Bio-Chemistry*”, by E.E. Conn & Stumpf, John Wiley & Sons, New York, (2000).
2. “*Text Book of Bio-Chemistry*”, by West, Todd et.al, Oxford and & BH Manohar Publishers & Distributers.
3. “*Principles of Bio-Chemistry*” by White, Handler, Smith et.al.
4. “*Bio-Chemistry*”, by Lehninger, W.H. Freeman and Companies, USA.
5. “*Bio-Chemistry*” by L.Stryer and W.H.Freeman and Companies, USA..
6. “*Organic Chemistry*”, by R.T.Morison and R.N.Boyd, Allyn & Bacon Inc., (printed in Singapore) (2001).



(PH24BC208) SUPRAMOLECULAR CHEMISTRY

Unit-1. Introduction

What is supramolecular chemistry? Selectivity, The 'Lock and Key' Principle and Induced Fit Model, Complementarity, Cooperativity and the Chelate Effect Preorganisation, Binding Constants, Kinetic and Thermodynamic Selectivity, Solvation Effects, Supramolecular interactions, Ionic and dipolar interactions, Hydrogen bonding, π interactions, Van der Waal's interactions, Close packing in the solid state, Hydrophobic effects, Supramolecular design.

Unit 2. Solution Host–guest Chemistry

Introduction: Guests in solution, Macrocyclic versus acyclic hosts, High Dilution Synthesis, Template synthesis, synthesis of 18-crown-6, 2.2.2.cryptand, calix[4]arene, thiacalix[4]arene, spherands, Cation binding, Crown Ethers, Lariat Ethers, Cryptands, Spherands, Calixarenes, Spherulates. Anion binding, Charged Receptors, Electrostatic Interactions, Electrostatic and Hydrogen Bonding Interactions, Neutral Receptors, Hydrogen-Bonding Interactions, Ditopic receptors, Neutral- molecule binding, Supramolecular catalysis and enzyme mimics, Calix[4]arenes and Cyclodextrins as catalysts. Use of spectral techniques like UV and fluorescence in analytical sensing

Unit 3. Supramolecular Polymers, Gels and Fibres: Introduction, Dendrimers, Covalent Polymers with supramolecular properties, self-assembled supramolecular polymers, polycatenanes and polyrotaxanes, supramolecular gels, polymeric Liquid crystals.

Unit 4. Supramolecular Devices

Introduction, Supramolecular Photochemistry, Information and Signals: Semiochemistry and Sensing, Molecule - Based Electronics, Photochemical devices, Molecular Wires and Rectifiers, Molecular Switches, Molecular Muscle, Towards Addressable Nanodevices, Nonlinear Optical Materials.

Unit 5. Supramolecular Chemistry of Nanomaterials

Nano-capsules and containers. Discussion of main synthetic strategies for their preparation. Examples of each type. Potential uses of such assemblies as nano-reactors and for transport (e.g. drug-delivery). Molecular switches and machines. Use of supramolecular forces to assemble components that respond (on-off) to external stimuli. Molecular shuttles, abacus

and muscles. Assembling such components into surfaces for molecular electronics. –
Supramolecular chemistry of polymeric materials and in the solid state. Self- assembled
monolayers. Molecularly imprinted polymers

Books:

1. Supramolecular Chemistry, 2nd Edition, March 2009 by Jonathan W. Steed Jerry L. Atwood
2. Core Concepts in Supramolecular Chemistry and Nanochemistry by J. W. Steed, D. R. Turner and K. J. Wallace, Wiley, 2007,
3. Chem. Rev. 2010, 110 (4), pp 1960–2004.
- 4 Bertini, H.B.Gray, S.J.Lippard and J.S.Valentine, Bioinorganic Chemistry, University Science Books, Sausalito, CA, USA, 1998.
5. J.M.Lehn, Supramolecular Chemistry – Concepts and Perspectives, VCH, Weinheim, 1995.
6. P.D.Beer, P.A.Gale and D.K.Smith, Supramolecular Chemistry. Oxford University Press, Oxford, 1999.

(PH24BC209) CHEMISTRY OF ENERGY SYSTEMS

UNIT-1: Electrochemical Systems: Galvanic cell, standard electrode potential, application of EMF, electrical double layer, dipole moments, polarization, Batteries-Lead-acid and Lithium ion batteries, super capacitors.

UNIT-2: Fuel Cells: Fuel cell working principle, Classification of fuel cells, Polymer electrolyte membrane (PEM) fuel cells, Solid-oxide fuel cells (SOFC), Fuel cell efficiency, Basic design of fuel cell.

UNIT-3: Hydrogen Storage: Hydrogen Storage, Chemical and Physical methods of hydrogen storage, Hydrogen Storage in metal hydrides, metal organic frame works (MOF), Carbon structures, metal oxide porous structures, hydrogen storage by high pressure methods. Liquefaction method.

UNIT-4: Solar Energy: Solar energy introduction and prospects, photo voltaic (PV) technology, concentrated solar power (CSP), Solar Fuels, Solar cells.

UNIT-5: Photo and Photo electrochemical Conversions: Photochemical cells and applications of photochemical reactions, specificity of photo electrochemical cell, advantage of photoelectron catalytic conversions.

References :

1. Physical chemistry by Ira N. Levine
2. Essentials of Physical Chemistry, Bahl and Bahl and Tuli.
3. Inorganic Chemistry, Silver and Atkins
4. Fuel Cell Hand Book 7th Edition, by US Department of Energy (EG&G technical services and corporation)
5. Hand book of solar energy and applications by Arvind Tiwari and Shyam.
6. Solar energy fundamental, technology and systems by Klaus Jagar et.al.
7. Hydrogen storage by Levine Klebonoff

(PH24BC210) CHEMISTRY OF POLYMERS AND THEIR APPLICATIONS

Unit – 1 : Polymers-Basics and Characterization

Basic concepts: monomers, degree of polymerization, linear, branched and network polymers, classification of polymers, Polymerization: condensation, addition and copolymerization, Mechanism of free radical, chain, ionic and coordination polymerization. Average molecular weight concepts: number, weight, viscosity average molecular weights, polydispersity and molecular weight distribution.

Measurement of molecular weight: End group, viscosity, light scattering, osmotic and ultracentrifugation methods, analysis and testing of polymers.

Unit – 2 : Synthetic Polymers

Addition and condensation polymerization processes – Bulk, Solution, Suspension and Emulsion polymerization.

Preparation and significance, classification of polymers based on physical properties, Thermoplastics, Thermosetting plastics, Fibers and elastomers, General Applications.

Preparation, properties and applications of Polymers based on different types of monomers, Olefin polymers, Diene polymers, nylons,

Urea - formaldehyde, phenol - formaldehyde and melanine Epoxy and Ion exchange resins.

Characterization of polymers by IR, NMR, GPC and XRD.

Unit – 3 : Natural Polymers & Modified cellulotics

Natural Polymers: Chemical & Physical structure, properties, source, important chemical modifications, applications of polymers such as cellulose, lignin, starch, rosin, shellac, latexes, vegetable oils, gums and proteins.

Modified cellulotics: Cellulose esters and ethers such as Ethyl cellulose, CMC, HPMC, cellulose acetals, Liquid crystalline polymers; speciality plastics- PES, PAES, PEEK, PEAK.

Unit-4: Hydrogels of Polymer networks and Drug delivery

Definitions of Hydrogel, polymer networks, Types of polymer networks, Methods involved in hydrogel preparation, Classification, Properties of hydrogels, Introduction to drug to drug delivery systems including, drug development, regulation, absorption and disposition, routes of administration and dosage forms. Advanced drug delivery systems and controlled release. Applications of hydrogels in drug delivery.

Unit – 5 : Surface phenomena

Surface tension, adsorption on solids, electrical phenomena at interfaces including electrokinetics, micelles, reverse micelles, solubilization. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

References :

1. A Text book of Polymer science, Billmayer
2. Organic polymer Chemistry, K.J.Saunders, Chapman and Hall
3. Advanced Organic Chemistry, B.Miller, Prentice Hall
4. Polymer Chemistry – G.S.Mishra
5. Polymer Chemistry – Vasant R. Gowariker, N. V. Viswanathan, Jayadev Sreedhar
6. Physical Chemistry –S. Glasston & K.J Laidler
7. Drug Delivery- Ashim K. Misra