COURSE STRUCTURE AND SYLLABUS

M.Sc (ANALYTICAL CHEMISTRY)

CHOICE BASED CREDIT SYSTEM (CBCS)

(With effect from 2022-2023)

CENTRE FOR CHEMICAL SCIENCES AND TECHNOLOGY

UNIVERSITY COLLEGE OF ENGINEERING, SCIENCE AND TECHNOLOGY, HYDERABAD (UCESTH)

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY HYDERABAD

KUKATPALLY, HYDERABAD-500085, TELANGANA

CENTRE FOR CHEMICAL SCIENCES & TECHNOLOGY (CCST)
M.Sc ANALYTICALCHEMISTRY
COURSE STRUCTURE

I YEAR

Subject Code	I semester	Course Title	Int. Marks	Ext. marks	L	P	C
1ACPC101	Program Core I	Organic Chemistry – I	40	60	3	-	3
1ACPC102	Program Core II	Inorganic Chemistry	40	60	3	-	3
1ACPC103	Program Core III	Physical Chemistry-I	40	60	3	-	3
1ACPE104	Program Elective I	(i) Principles of Analytical Chemistry (ii) Bio Molecules	40	60	3	-	3
1ACOE105	Open Elective I	(i) Applied Chemistry (ii) Computers and mathematics	40	60	3	-	3
1ACL106	Laboratory I	Inorganic Chemistry Lab	40	60	-	6	3
1ACL107	Laboratory II	Physical Chemistry Lab-I	40	60	-	6	3
1ACS108		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

Subject Code	II semester	Course Title	Int. Marks	Ext. Marks	L	P	C
2ACPC209	Program Core IV	Concepts in Organic Chemistry	40	60	3	-	3
2ACPC210	Program Core V	Instrumental Methods of Analysis	40	60	3	-	3
2ACPC211	Program Core VI	Physical Chemistry-II	40	60	3	-	3
2ACPE212	Program Elective II	(i) Spectroscopic Methods of Analysis- I (ii) Applied Analysis	40	60	3	-	3
2ACOE213	Open Elective II	(i) principles of chemical engineering (ii) Physical Organic Chemistry	40	60	3	-	3
2ACL214	Laboratory III	Organic Chemistry Lab –I	40	60	-	6	3
2ACL215	Laboratory IV	Physical Chemistry Lab-II	40	60	-	6	3
2ACS216		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

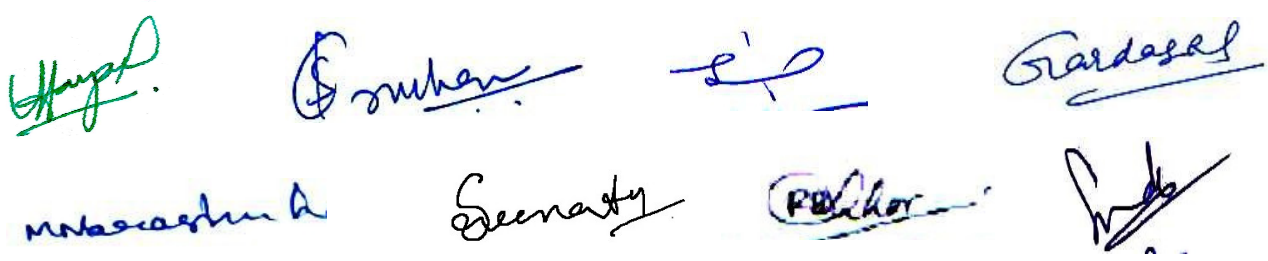
II YEAR

Subject Code	III semester	Course Title	Int. Marks	Ext. Marks	L	P	C
3ACPC317	Program Core VII	Quality Management and IPR	40	60	3	-	3
3ACPC318	Program Core VIII	Separation Methods	40	60	3	-	3
3ACPC319	Program Core IX	Spectroscopic Methods of Analysis II	40	60	3	-	3
3ACPE320	Program Elective III	(i) Hyphenated & Other Analytical Techniques (ii) Medicinal Inorganic Chemistry	40	60	3	-	3
3ACOE321	Open Elective III	(i) Food Technology, Pharmaceutical & Environmental Analysis (ii) Laboratory Analysis and management	40	60	3	-	3
3ACL322	Laboratory V	Wet Analysis Lab	40	60	-	6	3
3ACL323	Laboratory VI	Analytical Instrumentation Lab	40	60	-	6	3
3ACS324		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

Subject Code	IV Semester	Int. Marks	Ext. Marks	L	P	C
	Dissertation work review I	**0**	0	0	0	0
4AC425	Dissertation work review II	50	-	-	4	2
4AC426	Dissertation Evaluation (Viva Voce)	-	100	-	18	9
	Total	**50**	**100**		**22**	**11**

Total Marks: 750+750+750+150=2400

Total Credits: 23+23+23+11= 80



SEMESTER-I

PROGRAM CORE –I

1ACPC01: ORGANIC CHEMISTRY – I

UNIT – I: **Reaction Mechanism-I** (12 Hrs)

Addition Reactions:
Addition to carbon – carbon and carbon-hetero atom multiple bonds – Electrophilic, Nucleophilic and Free radical addition. Stereochemistry of addition to carbon – carbon multiple bonds, orientation and Reactivity.

Substitution reactions:
Aliphatic Nucleophilic substitutions – SN^1, SN^2 & SN^i mechanism, effect nucleophile, leaving groups, and solvent effect. Stereochemistry of nucleophilic substitution reactions, substitution at vinylic and allylic carbons, neighboring group participation. Aromatic nucleophilic substitution – mechanism – effect of substrate, structure, leaving group and nucleophile. Aromatic electrophilic substitution – reactions and mechanism.

Elimination reactions:
E_1, E_2, E_1CB. Elimination versus substitution reactions, pyrolytic syn-eliminations.

UNIT II: Stereochemistry-I (12 Hrs)

Concept of Chirality:
Molecular representation of organic molecules Wedge, Fischer, Newman and Sawhorse formulae, description and interconversion. Stereoisomerism, definition and Classification of Molecules based on symmetry and chiral center, Desymmetrization. Configurational nomenclature (DL&RS) Geometrical Isomerism – Cis/Trans and E/Z. Introduction to conformational Isomerism, Dynamic stereochemistry of Ethane, 1,2 Di-substituted ethane, Butane, Dihalo butanes, Halo hydrines, Ethylene glycol, Butane 2,3 diol, Amino alcohols, 1,1,2,2-tetra halo butanes. Cyclohexane and mono & di-substituted cyclo-hexane systems.

UNIT – III: Heterocyclic compounds I (12 Hrs)

Importance of heterocyclic compounds, classification and nomenclature of heterocyclic compounds, with one Hetero atom – General methods of synthesis, physical and chemical properties & applications of Furan, Pyrrole, Thiophene and their comparative reactivity. Benzothiophene, Indole, Benzofuran, Pyridine, Quinoline, Isoquinoline, Acridine, Carbazole, Coumarin and Chromone.

UNIT – IV Carbohydrates and vitamins: (12 Hrs)
Reactions of monosaccharides. Relative and absolute configuration of D (+)-Glucose and D (-)-Fructose. Determination structure of sucrose, maltose, lactose and cellobiose. Structural features of polysaccharides like cellulose and starch.
Vitamins: Classification of vitamins and applications of vitamins A_1, B_1, B_2, B_6, C, Biotin and E.

UNIT – V Reaction Intermediates and Rearrangements (12 Hrs)

a) Reactive Intermediates: Formation, stability and reactions of carbonium ions, carbanions, carbenes, free radicals, nitrenes and arynes

b) Molecular rearrangements

Definition and classification. Molecular rearrangement involving (i) Electron deficient carbons (Wagner – Meerwein, Pinacol-Pinacolone) (ii) Electron deficient Nitrogen (Hofmann, Curtius, Lossen, Beckmann, Schmidt) (iii) Electron deficient Oxygen (Baeyer – Villiger). Base Catalyzed rearrangements (Benzillic acid, Trans annular, Von Richter, Sommlett - Hauser and Smiles).

Suggested books:

1. Stereochemistry of Organic Compounds by Ernest L. Eliel, Samuel H. Wilen.
2. Stereochemistry of organic compounds: Principles and Applications by D. Nasipuri.
3. Heterocyclic Chemistry by T.L. Gilchrist.
4. Organic Chemistry by RT Morrison and RN Boyd.
5. Organic Chemistry, Vol. 2 by I.L. Finar.
6. Organic Chemistry by Clayden.
7. Heterocyclic Chemistry by J.A.Joule, K.Mills and G.F.Smith.
8. Organic Reaction Mechanisms by V.K. Ahluwalia & Rakesh K. Parashar.

Further reading:

1. Benzofurans by A. Mustafa.
2. The Chemistry of Indole by R. J. Sunderberg.
3. An introduction to the chemistry of heterocyclic compounds by R.M.Acheson.
4. Advanced Organic Chemistry: Reactions, Mechanisms and Structure by Jerry March
5. Reaction Mechanism In Organic Chemistry By Mukherjee And Singh
6. Guide Book to mechanism in Organic Chemistry by Peter Sykes.
7. Organic Chemistry by Graham Solomous and Craig B Fryhle
8. Organic Chemistry: Structure and Reactivity by Ege, Seyhan N.

SEMESTER-I

PROGRAM CORE –II

1ACPC02: INORGANIC CHEMISTRY

UNIT – I: Coordination and Bio Coordination chemistry (12 Hrs)

Crystal Field Theory: d-Orbital splitting patterns in Octahedral (regular, compressed and elongated), Square Pyramidal, Trigonal bipyramidal, Tetrahedral, square planar, Trigonal planar and Linear geometries, Factors influencing the magnitude of Crystal Field Splitting in Octahedral Complexes –Spectrochemical series of ligands - concept of weak and Strong crystal Fields-Calculation of Crystal Field Stabilization Energies (CFSE) in Six and Four –Coordinate Complexes– High Spin – Low Spin - Limitations of CFT Model for Complexes - Experimental Evidence for Metal-Ligand Bond Covalency Thermodynamic aspects of Crystal Field splitting.

Metal Ions in Biological Systems:

Brief Survey of Metal Ions in Biological Systems –Effect of Metal Ion Concentration – Basic Principles Underlying Biological Selection of Elements. Oxygen Transport and Storage:Haemoglobin and Myoglobin, Geometric, Electronic and Magnetic Aspects of Dioxygen Binding, Oxygen Adsorption Isotherms and cooperativity in Haemoglobin and its physiological significance, role of the Globia Chain.

UNIT – II: Coordination Equilibria (12 Hrs)

Solvation of Metal Ions –Binary Complexes: Formation of Binary Metal Complexes and their Stability-Types of Stability Constants: Thermodynamic, Concentration and Conditional Constants –relationship between stepwise and overall stability constants – Trends in Stepwise stability Constants - Factors influencing the Stability Constants: i) Ligand Effects: Basicity, Substituent, Steric, Chelate (Size and Number of Chelate Rings), Macrocyclic and Cryptate Effects ii) Metal Ion Effects : Ionic Potential, Effective Nuclear Charge and Atomic Number (Irving's –William's Order, Geometry of Metal Ion and Ligand) Chelate Effect and its Thermodynamic Origin, Jahn–Teller Effect on Stability Constants of Metal Complexes – Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electro negativity Vs Hardness and Softness.

UNIT – III: Reaction Mechanism: (12 Hrs)

Energy profiles of reaction - Reactivity of metal complexes: Inert and labile complexes, Concept of Liability and Inertness in terms of valence bond and crystal field theories.

Nucleophilic Substitution reactions of Octahedral Complexes:

Dissociative and Associative Mechanisms-Mechanistic labels-In gold's Terminology (SN^1 and SN^2) Long Ford-Gray Terminology-Acid hydrolysis, Factors effecting acid hydrolysis,

Base hydrolysis-conjugate Base Mechanism-Evidence in favor of conjugate mechanism. Reactions without Metal-Ligand Bond cleavage.

Nucleophilic Substitution Reactions of Square planar Complexes*:*

Mechanism of substitution in square planar complexes. Evidence in favor of Associative Mechanism –Trans Effect, Theories of Trans effect-Applications of Trans effect.

Electron – Transfer reactions:
Inner & outer Sphere Electron Transfer Reaction mechanisms, Marcus-Hush Theory.

UNIT – IV: Molecular symmetry and Group Theory: (12 Hrs)
Concept of Symmetry in Chemistry – Symmetry Operations – Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry, Inversion Center and Identity Element –Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification Molecules in to C_1, Cs, C_i , C_n,C_{nv}, C_{nh}, $C_{\infty v}$, D_n, D_{nh}, D_{nd}, $D_{\infty h}$, S_n (n=even), T_d, O_h, I_h, K_h Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity. Term symbols.

UNIT – V: Metal Clusters (12 Hrs)
Carbonyl Clusters
a) Ligational properties of CO:Donor (HOMO) and Acceptor (LUMO) Molecular Orbitals of CO Bonding modes of CO: Terminal and Bridging-Bonding - Classification into mononuclear, Binuclear, Trinuclear and Tetranuclear carbonyls. Structures of Ni $(CO)_4$, Cr $(CO)_9$, $Mn_2(CO)_{10}$, $Fe_2(CO)_9$and $Co_2(CO)_8$-Eighteen Electron Rule in Metal Carbonyls.
b) Factorsfavoring Metal-Metal Bonding-Classification of Clusters**.** Structures and bonding in Carbonyl clusters. $M_4(CO)_{12}$ M=Co, Rh, Cr. $M_3(CO)_{12}$, M=Fe
c)Metal halide clusters:
Major structural types in Dinuclear Metal-Metal systems. Structure and Bonding in Halides of Mo(II) and Re(III).

Suggested Books:

1. F.A.Cotton and Wilkinson: Advances in inorganic Chemistry, 1989.
2. J.E.Huheey : Inorganic chemistry, 1983.
3. J.D.Lee :Concise Coordination chemistry.
4. Symmetry & Spectroscopy of Molecules K.Veera Reddy,New Age international Ltd 1998.
5. Selected Topics in Inorganic chemistry madan,Malik,Tuli S.Chand publications.

Further reading:

1. BioInorganic Chemistry- K.Hussain Reddy
2. Inorganic reaction Mechanism- F.Basolo & R.G.Pearson, New York.
3. Inorganic Chemistry- Keith F.Purcell & John C.Kotz Holt- Saunde International Edition.
4. Ligational aspects of diatomic molecules-Organometallic Chemistry R.C.Mehotra.

SEMESTER-I

PROGRAM CORE –III

1ACPC03: PHYSICAL CHEMISTRY – I

UNIT- I: Thermodynamics-1 (12 Hrs)

Brief review of concepts and the I and II laws of Thermodynamics. Concept of entropy-entropy as state function. Entropy changes in various processes. Entropy changes in ideal gas. Entropy change on mixing of ideal gases. Entropy as a function of V & T. Entropy as a function of P& T. Entropy changed in isolated systems - Clausius inequality. Entropy change as criterion for spontaneity and equilibrium.

Third law of thermodynamics:

Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Helmholtz and Gibbs energies (A&G). A&G as criteria for equilibrium and spontaneity. Physical significance of A&G. Driving forces for chemical reactions-relative signs of ΔH & ΔS.

Thermodynamic relations:Gibbs equations. Maxwell relations. Temperature dependence of Gibbs Helmholtz equation. Pressure dependence of G. Phase equilibrium. Clapeyron equation and Clausus-Clapeyron equation.

Unit-II: Electrochemistry (12 Hrs)

Ionics:

Terminology of Conductance, ohm's law electrolytic conductance, Kohlrausch's law and its applications ionic equilibria, conductometric titrations.

Debye – Huckel theory: Debye – Huckel theory of strong electrolytes, Activity coefficients of electrolytes. The Debye – Huckel limiting law (DHLL)

Electrodics:

Types of electrodes, Electrode potentials, electrode reaction-Nernst equation and its derivation. Cell EMF. Reference electrodes, Indicator electrodes, Chemical cells and Concentration cells, with and without transference. Potentiometric titrations-determination of pH and Solubility product from EMF measurements.

Unit-III: Quantum chemistry (12 Hrs)

Basic Principles: Black body radiation-Planck`s concept of quantization-Planck`s equation (derivation not required). Photoelectric effect, Hydrogen spectrum. Bohr`s theory and its failures. Wave-Particle duality and uncertainty principle-significance of these for microscopic entities. Emergence of quantum mechanics.

Operators: operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators Δ and Δ_2. Eigen functions and Eigen values. Degeneracy. Linear Combination of Eigen functions of an operator. Well behaved functions. Normalized and Orthogonal functions.

Postulates of Quantum mechanics*:* Physical interpretation of wave functions. Observables and Operators. Measurability of properties. Particle in a box and explain wave function and energy in the system.

UNIT IV: Chemical Kinetics (12 Hrs)

Theories of reaction rates

Collision theory, steric factor, Transition state theory, Reaction coordinate, Activated complex and the transition state. Thermodynamic formulation of transition state theory. Activation parameters and their significance. The Eyring equation, Unimolecular reactions and Lindamann's theory. Salt effects.

Complex Reactions

Opposing reactions, parallel reactions, consecutive reactions (all first order type). Chain reactions, chain length, Rice Herzfeild Mechanism, explosion limits general Characteristics, Steady state treatment. Ex: H_2-Br_2 reaction, Derivation of rate law.

Homogeneous catalysis

Introduction to homogeneous and heterogeneous catalysis with examples in homogeneous catalysis.

Introduction to enzyme catalysis: Michaeli's -Menten kinetics.

UNIT V: Solid State Chemistry (12 Hrs)

Crystalline nature

Classification. Crystal defects. Perfect and imperfect crystals. Classification of imperfections. Point defects. Schottky defects. Frenkel defects. Line defects and plane defects. Electron diffraction, Bragg's law and applications, Band theory, band structure of metals, insulators and semiconductors.

Superconductivity. Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect. Types of superconductors. Theories of super conductivity-BCS theory, high temperature superconductors.

Suggested Books:

1. Introduction to chemical thermodynamics – by I.M.Klotz
2. Introduction to chemical thermodynamics – by R.P.Rastogi,R.R.Misra
3. Chemical Kinetics by K.J.Laidler
4. Chemical Kinetics by C.Kalidas or J.C.Kuriakose

Further reading:

1. Quantum Chemistry,R.K.Prasad Wiley Eastren,New Delhi.
2. Quantum Chemistry by D.A.Mc Quarrie,University science books ,Mil valley, california
3. Solid State Chemistry, K.F.Purcell and J.C. Klotz
4. Solid State Chemistry,A.R.West,John Wiley, 1990

SEMESTER-I

PROGRAM ELECTIVE- I

1ACPE04.1: PRINCIPLES OF ANALYTICAL CHEMISTRY

UNIT-I: Data Handling (12 Hrs)

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student's t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.

UNIT-II: Gravimetric analysis and titrimetric analysis (12 Hrs)

Gravimetric analysis: Principles of precipitation gravimetry; Nucleation, precipitation, and growth of precipitates; Particle size and filterability of precipitates; Precipitation from homogeneous solution; Co precipitation - impurities in precipitation, Washing, drying, incineration of precipitates; Use of organic reagents in Gravimetric analysis

Titrimetric Analysis

Principles underlying titrimetric methods; Equivalence point and endpoint; detection of end point.

Types of titrations.

i) Redox titrations:

Principle and detection of equivalence point by visual & potentiometric methods. Applications - Use of Jones reductor; Karl Fisher reagent for water determination.

ii) Complexometric titrations:

Principles of complexometric titrations, stability constants, Use of EDTA for the determination of metals and practical considerations.

UNIT-III: **Chemical Analysis and GLP** (12 Hrs)

Practical Aspects of Chemical Analysis: Analysis of real samples - Choice of analytical method; Literature survey; Analysis of standard samples; Preparing samples for analysis – preparing laboratory samples; moisture in samples; drying the analytical sample; decomposition and dissolution of sample and source of errors in decomposition and dissolution

Good laboratory practices and implementation: Equipment's, Quality assurance practices, SOPs, reagents, solutions, test and controls, raw data analysis and GLP practices

UNIT-IV: Chromatographic techniques -1 (12 Hrs)

Fundamentals of chromatographic separation methods – Definition, Principles of chromatography, sorption mechanisms - differential migration, partition and adsorption phenomena; Classification of different chromatographic methods; Methods of development- Elution development, Gradient elution development, displacement development and frontal

analysis. *Dynamics of chromatography*-efficiency of chromatographic column, zone spreading, Height Equivalent to Theoretical plate (HETP).

Column chromatography:
principles, general aspects, adsorption isotherms, chromatographic media, nature of forces between adsorbent and solutes, eluents, (mobile phase), column chromatography without detectors and liquid chromatography with detectors and applications.

UNIT-V: Chromatographic techniques -2 (12 Hrs)
Paper chromatography:
principle, papers as a chromatographic medium, modified papers, solvent systems, mechanism of paper chromatography, experimental technique, different development methods-ascending, descending, horizontal, circular spreading, multiple development, two-dimensional development, reverse phase paper chromatographic technique visualization and evaluation of chromatograms, applications.

Thin Layer Chromatography: (12 Hrs)

principle, chromatographic media-coating materials, applications, activation of adsorbent, sample development, solvent systems, development of chromatoplate, types of development, visualization methods, documentation, applications in the separation, HPTLC principle, technique, applications.

Suggested books:

1. Douglas A. Skoog, Donald M. West and F. James Holler, analytical chemistry an introduction, saunders college publishing, New york, 1990.
2. J. Bassett, R.C. Denny, G. Jeffery and J. Mendham. Vogel's text book of inorganic Quantitative analysis, 4th edition, Longman group Ltd, Harlow, 1985.
3. Pietrazyk and Frank. Analytical chemistry, 1990.
4. KVSG Muralikrishna, An Introduction to ISO 14000, Environmental Management, 1998.

Further reading:

5. Y. Anjaneyulu, Quality Assurance and GLP – IGNOU Pub., New Delhi, 1999.
6. Omachonu V.K.and Ross J.E. Principles of Total quality, S. Chand & Co.Ltd., New Delhi, 1997.
7. Werner Funk, Vera Damman, Gerhild Donnervert. Quality Assurance in Analytical Chemistry, VCH Publishers, New York, NY (USA), 1997.
6. Bertamd L. Hanser and Prabhakar Ghani. Quality Control and Applications, Prentice-Hall

SEMESTER-I

PROGRAM ELECTIVE- I

1ACPE04.2: BIOMOLECULES

UNIT-I. Enzymes & Proteins: (12 Hrs)

Classification of Amino acids Primary, secondary and tertiary structure of Proteins, Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three-point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilized enzymes.

UNIT-II. Nucleic acids: (12 Hrs)

Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleosides and nucleotides, Watson –crick model of DNA, different base pairing.

UNIT-III. Lipids-Oils and Fats: (12 Hrs)

Classification, role of lipids, fatty acids and glycerol derived from oils and fats; Physical properties - polymorphism, reactions of fats, rancidity, reversion, polymerization, saponification, addition, hydrogenation, phospholipids, lipid metabolism; intermediary metabolism of fatty acids, synthesis of fatty acids.

UNIT-IV: Vitamins: (12 Hrs)

Classification, distribution in foods, loss during processing, effects of deficiency and characteristic properties of vitamins – B1(Thiamine), B2(Riboflavin), B3 (Pantothenic acid),B_6 (pyridoxine), B12 (Cyanocobalamine), H(Biotin), P(Rutin) C(ascorbic acid) A(Retinol) D(Calciferol), E(Tocopherol) K(naphthoquinone).

UNIT-V: Introduction to Drugs (12 Hrs)

Introduction, Classification, examples of natural and synthetic drugs

Chiral drugs: Introduction to chiral drugs. Synthesis and pharmacological activity of S-Ibuprofen, S- Metaprolol, Ininavir sulfate, Levocetirizine, 2S-Verapamil, S, S-Ethambutol, (+) Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+) Ephedrine, (+) Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S, S- Captopril and S,S,S- Enalaprilate

Suggested books:

1. Enzyme structure and mechanism by Fersht and Freeman
2. Bio-Organic chemistry by Hennan Dugas
3. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
4. Lehninger Principles of Biochemistry by D L Nelson and M Cox
5. Outlines of Biochemistry by Conn and Stumpf

Further reading:

1. Biotransformations in Organic Chemistry by K Faber.
2. Principles of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.

SEMESTER-I

OPEN ELECTIVE- I

1ACPOE05.1: APPLIED CHEMISTRY

UNIT-I: Nano materials (12 Hrs)

Introduction to Mesoporous materials, Nano-sized materials, Crystal structure, properties of individual Nano particles, Metal Nano Clusters, Preparation techniques like hydrothermal synthesis, sol-gel processes, Hard templating routes, Rf plasma chemical methods, Thermolysis and pulsed laser methods, *In situ* reduction methods, Carbon nanotubes, fullerenes, graphene, their synthesis, characterization & applications, characterization by XRD, SEM, TEM.

UNIT-II: Purification Techniques (12 Hrs)

a) Methods of Purification:

Purification, List of Purification Methods

Distillation: Basic principles. Distillation types, continuous distillation, batch distillation, fractional distillation, vacuum distillation and steam distillation. Deans-stork Distillation and their Industrial applications.

Types of Solvents: Different types of solvents based on polarity, Chemical Nature

Drying Techniques: Drying of Hexane, Benzene, Toluene, Xylene, Tetrahydrofuran, DMF, DMSO, Methanol, Ethanol, Diethyl ether, Dioxane

CrystalizationTechniques: Different kinds of crystallization, Single crystal generation b) **Industrial safety:**

Introduction, Factors Contributing to the Costs of Accidents, List of some Notable accidents in the process industry/selected case histories. **Material hazards**: Introduction Hazards substances-categories, Toxicity, Radiation, Flammability, Ignition, Fires and explosions.

UNIT-III: Water Technology & Corrosion (12 Hrs)

Hardness of water – Temporary and permanent Hardness- units. Desalination of Brackish water-Reverse Osmosis and Electro dialysis. Industrial treatment of water- Lime soda ash method-Chemical reaction- problems- zeolite and ion exchange process. Boiler troubles- scale and sludge formation – Caustic Embrittlement and boiler corrosion- Internal conditioning methods-phosphate and carbonate conditioning- priming and Foaming.

Corrosion-Causes and effects of corrosion – theories of chemical and electrochemical corrosion –mechanism of electrochemical corrosion, Types of corrosion: Galvanic, water-line and pitting corrosion. Factors affecting rate of corrosion, Corrosion control methods- Cathodic protection – Sacrificial anode and impressed current cathodic methods. Surface coatings – metallic coatings – methods of application. Electroless plating of Nickel.

UNIT IV: Fuel Technology (12 Hrs)

Classification of fuels, characteristics of fuels-calorific value units (lower, higher) and its determination-Bomb calorimetric method. Solid fuels - classification of coal, Rank analysis of coal - proximate and ultimate analysis.

Liquid fuels-Introduction, origin of petroleum, classification-mining, refining, cracking (thermal and catalytic), synthesis and purification of gasoline-knocking and octane number of gasolines, Diesel - Cetane number-high speed and low speed diesel oil. Gaseous fuels-biogas, LPG. Analysis of fuel gases.

UNIT-V: Polymer Chemistry & Engineering Materials (12 Hrs)

Types of polymerization –anionic, cationic, free radical, coordinate polymerization ring opening. Types of initiators-Free radical, Anionic, Cationicpolymerizations. Molecular weight of polymers $M_{W,\ Mn}$determination osmometry, light scattering basics of kinetics of polymerization.
Preparations and applications of the following
i)polyethylene, polystyrene, polyvinyl chloride, silicone resins.
ii)synthetic fibers: Nylon 66, Dacron, orlon, Rayon.
iii)Rubbers, Elastomers.
iv)conducting polymers, Biodegradable polymers.
Ceramics-Introduction-Classification – Glazed &Unglazed Ceramics -Properties-**Applications**
Lubricants-Definition and Explanation of Lubrication-Mechanism of Lubrication –Types of Lubricants -Properties of Lubricants-Engineering applications.

Suggested Books:

1. A Textbook of engineering chemistry –Jaya Shree Anireddy. Wiley precise textbook series, Wiley India Pvt.Ltd, 2018
2. A Text book of engineering chemistry –S.S.Dara& K.Mukkanti,
3. Applied Chemistry-II, V.M. Balsaraf, I.K.International.
4. Applied Chemistry, H.D. Gesser, Springer.

Further reading:

1. Comprehensive engineering chemistry-Devender singh, Balsaraf, Satish KumarVats,
2. I.K.International.
3. Chemical process industry safety by K S N Raju, Mc Graw Hill Education, 2014
4. Nanotechnology in Catalysis by Pinzhan
5. Springer Handbook of Nanotechnology by Bharat Bhushan
6. Introduction to Polymer Chemistry by Charles E.Carraher.
7. Textbook of Polymer Chemistry by Man P Singh.
8. Organic Chemistry by Marye Anne Fox, James K. Whitesell

SEMESTER-I

OPEN ELECTIVE- II

1ACPOE05.2: COMPUTERS AND MATHEMATICS

UNIT-I: Computer basics: (12 Hrs)

Problem solving using computers- flowcharts-algorithms-CPU-Input and output units-.computer memory- Basic concepts of Object oriented Languages Basic structure of C++ programming-tokes-keywords-data types: basic data types-derived data types-user defined data types-constants-variables-arrays-one, two and multi dimensional arrays-structure-union-enumerated data types.

UNIT-II: Arithmetic operators: (12 Hrs)

Relational operators-increment and decrement operators-bit wise operators-arithmetic expression-precedence of operators-Evaluation of expression- type compatibility-expression and implicit conversion-manipulators-control structures: decision making and branching-decision making and looping-Function declaration and definition- argument passing-return values.

UNIT-III: Classifications: (12 Hrs)

Class and objects-member functions- array of objects-object as an argument- function overloading- friend function-operator overloading-this pointer-static data member-static member function Constructors: default constructor-parameterized-copy constructor-dynamic constructor-destructors-Inheritance-single inheritance-multiple inheritance-multilevel inheritance-pointers virtual functions and polymorphism

Unit-IV: Differential Calculus: (12 Hrs)

Functions- continuity and differentiability, Rules for differentiation. Sums, products and quotients of functions. The chain rules. Differentiation of algebraic, exponential logarithmic and composite functions. First order differential equations- separable variables. Homogenous and linear differential equations. Linear second order differential equations- solutions for homogenous equations.

Higher order derivatives. Maxima and minima. Partial differentiation and meaning of total derivative exact and inexact differentials

Integral Calculus:

Basic rules for integration. Methods for evaluating integrals-the substitution method, use of partial fractions, integration by parts. Definite integrals.

UNIT V: Introduction to statistics (12 Hrs)

population-sample –primary data and secondary data - graphical and diagrammatic representation of data- Measure of central tendency-Mean, median and mode measure of dispersion-range-standard deviation. Binomial, Poisson and Normal distribution (definitions statements of properties and examples). Linear regression multi variant analysis DimensionalityReduction

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Suggested Books:

1) Fundamentals of Computers by V Raja Raman
2) Object Oriented Programming with C++ by E. Balagurusawmy
3) Statistical methods S.P.Gupta. S Chand Publications

SEMESTER-I

LABORATORY-I

1ACL06: INORGANIC CHEMISTRY LAB

Quantitative Analysis: Preparation of the following inorganic complexes.

a) Tetraammine Cu(II)sulphate.
b) Hexaammine Ni (II)chloride
c) Tris (ethylene diamine) Ni (II)thiosulphate.
d) Mercury tetra thiocyanato cobaltate II
e) Potassium tri oxalate chromate III
f) $[Co(NH_3)_5Cl]Cl_2$,
g) $[Co(NH_3)_5NO_2]Cl_2$,
h) $[Co(NH_3)_5ONO]Cl_2$

1. Estimation of Al^{+3} by back titration.
2. Estimation of Ca^{+2} by Substitution titration.
3. Estimation of Ba^{+2} Gravimetrically.
4. Determination of Cu^{+2} and Ni^{+2} in a mixture
5. Determination of Ca^{+2} and Mg^{+2} in a mixture
6. Determination of Ferrocyanide and Ferriccyanide.

Suggested Books

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe,2nd edn John Wiley & Sons.
3. Experimental Inorganic/Physical Chemistry, M. A. Malati, Horwood Publishing, Chichester, UK (1999)

SEMESTER-I

LABORATORY-II

1ACL07: PHYSICAL CHEMISTRY-LAB-I

Acid Base Titrations

Conductometry

1. Mixture of acids Vs Strong base
2. Verification of Ostwald's dilution law – dissociation constant of a weak acid

Potentiometry

1. Mixture of acids Vs Strong base
2. Relevance of PKa in defining acidity/ basicity of chemical entities

Chemical Kinetics

1. Hydrolysis of methyl acetate using HCl
2. Hydrolysis of methyl acetate using H_2SO_4
3. Hydrolysis of methyl acetate using HCl & H_2SO_4 compare the relative Strengths of the acid.
4. Determination of activation energy at two different temperatures
5. Investigate the Reaction between $Kmno_4$ and $C_2H_2O_4$ Auto catalitically
6. Investigate the Reaction Between Acetone And Iodine
7. Kinetics of Reaction between Potassium per sulphate and Potassium Iodide

Suggested Books:

1. Advanced Practical Physical Chemistry by J.B.Yadav.
2. Basic Practical physical chemistry by V.K.Ahulwalia
3. Practical physical chemistry by B.D.Khosla

SEMESTER-II

PROGRAM CORE IV

2ACPC08: CONCEPTS IN ORGANIC CHEMISTRY

Unit I: Principles of Stereochemistry (12 Hrs)

Relative and absolute configuration: Determination of absolute configuration –Racemisation, racemates and resolution techniques: resolution by direct crystallization, diastereomer salt formation, Chiral chromatography and asymmetric transformations. Methods of racemisation. Axial, planar and helical chirality, configurational nomenclature: Atropisomerism, Axially chiral biaryls, allenes, spiranes, ansa compounds and Helically chiral compounds. Conformational diasteromers & enantiomers, factors affecting conformational stability and conformational equilibrium-attractive and repulsive interactions.

Unit II: Formation of C-C and C=C bonds (12 Hrs)

-C-C- (Single) bonds: Alkylation importance of enolate ions - Alkylation of ketones – The enamine reaction and Lithium dialkyl cuprates. >C=C< (double) bonds: β elimination reactions. Pyrolytic synthesis, eliminations - Wittig and related reactions. Reactions of unactivated carbon-hydrogen bonds: Hofmann, Loffler, Freytag reaction, Barton reaction.

Unit III: Heterocyclic Compounds-II (12 Hrs)

Five and six membered heterocyclic systems with more than one heteroatom. Synthesis, properties and applications of Pyrazole, Imidazole, Benzimidazole, Purine, Pyrimidine, Oxazole, Isooxazole, Oxadiazole, Thiazole, Thiadiazole, Triazole, Tetrazole, Pyradazine, Pyrazine, Triazine.

Unit-IV: Photochemistry (12 Hrs)

Photo physical processes and photochemical processes. Electronically excited molecules-singlet and triplet states. Jablonski diagram. Photochemistry of carbonyl compounds - n– π^*, π – π^* transitions, Norrish type I and Norrish type II cleavages, Peterno-Buchi reactions, rearrangements of α,β,- unsaturated ketones and cyclic hexadienes, photochemistry of P-Benzoquinones, photochemistry of unsaturated system – olefins, cis-trans isomerism and addition acetylenes dimerisation, dienes – photochemistry of 1,3- butadienes (2+2) additions leading to cage structures and photochemistry of cyclohexadienes, Di-π methane rearrangement

Unit V: Pericyclic Reactions (12 Hrs)

Classification of pericyclic reactions into electrocyclic reactions; cycloaddition and sigmatropic reactions

Electrocyclic reactions: in 4n and 4n+2 electron system – Explanation of theory of electrocyclic reaction by 1) Huckel-morbius aromatic and antiaromatic transition method

2) Frontier molecular orbital method (Woodward-Hofmann selection rules)

3) conservation of orbital symmetry method (correlation diagrams method)

Cyclo addition and cyclo reversions:

$\pi + \pi^2$ and $\pi^4 + \pi^2$ cycloaddition reactions. Suprafacial, antarafacial interactions. Mention of characteristics of Diels-Alder reaction by Huckel-morbius Theory 2) HOMO-LUMO method

Sigmatropic reactions of the order [1, j]

Suprafacial and antarafacial shifts, explanation for the mechanism of sigmatropic reactions by 1) Huckel-morbius aromatic and antiaromatic transition method 2) HOMO-LUMO method – cope and claisen rearrangements

Suggested Books:

1. Stereochemistry of carbon compounds by Ernest L.Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
3. Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4. Heterocyclic Chemistry, 3rd Edn J.A.Joule, K.Mills and G..F.Smith.
5. Advanced Organic Chemistry by Jerry March
6. Pericyclic Reactions by Mukherjee S M
7. Photochemistry by C W J Wells

Further reading:

1. Mechanism and Structure in Organic Chemistry S. Mukerjee
2. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
3. Organic Chemistry by RT Morrison and RN Boyd.
4. Organic Chemistry, Vol. 2 by I.L. Finar.
5. Organic Chemistry: Structure and Reactivity by Seyhan Ege.
6. Conservation of Orbital Symmetry by Woodward and Hoffmann
7. Organic Photochemistry by Turro
8. Molecular Photochemistry by Gilbert & Baggo
9. Organic Photochemistry by D Coyle

SEMESTER-II

PROGRAM CORE V

2ACPC09: INSTRUMENTAL METHODS OF ANALYSIS

UNIT-I: **Advanced Chromatographic Techniques** (12 Hrs)

GC: Theory, Instrumentation - description of equipment and different parts, columns (packed and capillary columns), detector specifications –thermal conductivity detector, Flame ionization detector, electron capture detector, nitrogen-Phosphorous detector, photo ionization detector, programmed temperature gas chromatography, applications in the analysis of gases, petroleum products etc.

HPLC: Theory, Instrumentation - description of the different parts of the equipment, stationary phases (columns), mobile phase, detectors - UV detector, RI detector, Fluorescence detector, Photo Diode Array detector, ELSD, conductometric detector, and electrochemical detector, applications, advantages and disadvantages.

UNIT-II: Polarography and cyclic Voltammetry: (12 Hrs)

Basic principles, Instrumentation, Polarographic techniques, Application of polarography in quantitative analysis, analysis of mixtures, application to organic compounds, polarography of metal complexes**,** Amperometric titrations.polarography, rapid scan, pulse and square wave polarography, differential pulse polarography (DPP), cyclic voltametry, chronopotentiometry-basic principles, applications and advantages.

UNIT-III: Diffraction Techniques (12 Hrs)

I) **X- ray diffraction**: crystal structure, Miller indices, Bragg's equation, Structural analysis of crystals, powder diffraction, NaCl & KCl crystal structures.
II) Fundamentals of **Electron diffraction techniques**
III) Fundamentals of **Neutron diffraction techniques.**

UNIT-IV: Electrochemical methods of analysis-1: (12 Hrs)

Conductometry:
Principle, Fundamental equations, measurement of conductance, Conductometric titrations.

Potentiometry:
Principle, apparatus and technique, potential (emf),Nernst equation, reference electrodes, measurement of potential, applications to neutralization, redox, precipitation, complexometric titrations, location of end points, differential titrations, advantages of potentiometric titrations.

pH metry: Principle, Instrumentation, The Glass pH electrode – theory, construction, standard buffers, pH titrations.

UNIT-V: Electrochemical methods of analysis-2: (12 Hrs)

Metallic indicator electrodes: Electrodes of first kind, second kind and third kind metallic redox indicator, cell with and without liquid junction, reference electrodes. Ion selective indicators: Membrane indicator electrodes: classification of membranes, properties of ion-selective membrane, Glass membrane electrodes, precipitation electrodes, solid-state electrodes, liquid-liquid electrodes, plastic/ionophore electrodes, coat wire electrodes. Molecular – selective electrode systems: Gas – sensing probes, bio catalytic membrane (enzyme) electrodes: Mechanism of membrane response, the selectivity ratio, Ion selective evaluation methods, interferences – chemical and electrode interferences, applications of ion selective electrodes. Advantages and disadvantages.

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Suggested books:

1. R.A.Day & A.L.Underwood, Quantitative analysis, Prentice-Hall of India Pvt. Ltd.
2. Skoog & West, Fundamentals of Analytical Chemistry
3. Hobert H.Willard, D.L.Merrit & J.R.J.A.Dean, Instrumental methods of analysis, C.B.S Publishers and Distributors
4. Vogel, Textbook of quantitative inorganic analysis
5. Ewing, Instrumental Methods of Analysis
6. Instrumental Methodology of Analysis by Chatwal Anand.

SEMESTER-II

PROGRAM CORE VI

2ACPC10: PHYSICAL CHEMISTRY –II

UNIT- I: Thermodynamics-II (12 Hrs)

Ideal solutions: Thermodynamics properties of ideal solutions. Mixing quantities. Vapor pressure- Raoult`s law. Thermodynamic properties of ideally dilute solutions. Vapour pressure-Henry`s law.

Non ideal systems.Concept of fugacity, fugacity coefficient. Determination of fugacity. Nonideal solutions. Activity and activity coefficients. Standard-state conventions for Nonideal solutions. Excess functions and their determination.

Statistical thermodynamics: The distribution of molecular states-configurations and weights, The dominating configuration.Boltzmann distribution; Kinetic theory of gases. The molecular partition function, its interpretation and their relations to thermodynamic quantities, Sucker-Tetrode equation- calculations for model systems.

Unit-II: Polymers (12 Hrs)

Classification of polymers. Types of polymerization. Kinetics and mechanism of free radical polymerization. The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. The glassy state – glass transition temperature T_g of polymers.

Molecular weight distribution – measurement of molecular weights by osmometry

Smart materials – their uses in sensing devices and communication networks. Conducting polymers. Electrically conducting polymers and their uses

Ionic exchange polymers. Cationic and anionic exchange polymers and their uses. Eco-friendly polymers.

Membrane separation. Liquid separation – dialysis, electro osmosis and reverse osmosis.

UNIT-III: Photochemistry (12 Hrs)

Photo physical processes and photochemical processes. Electronically excited molecules-singletand triplet states. Jablonski diagram.Fluorescence emission and Phosphorescence emission. Quantum yield and determination.

Photochemical reactions with high and low quantum yields-examples. Transfer of excitation energy-Sensitization and quenching. Stern – Volmer equation

UNIT IV: Surface chemistry (12 Hrs)

Study of surface– Langmuir and BET adsorption isotherms-study of kinetics of surface reactions catalysis by metals, semiconductor oxides-mechanism of heterogeneous catalytic reactions-the adsorption coefficient and its significance.

Heterogeneous Catalysis: Catalytic activity at surfaces, Adsorption and catalysis – Eley-Rideal Mechanism, Langmuir-Hinshelwood mechanism. Examples of heterogeneous catalysis – Hydrogenation, Oxidation, Cracking and reforming.

Colloids: Types, preparation, Characterization of colloids. Colloids in industry.

UNIT V: Quantum Chemistry-II (12 Hrs)

Particle in a box- one dimensional and three dimensional. Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

Cartesian, Polar and spherical polar coordinates and their interrelations

Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams.

Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations.

Suggested Books:

1. Advanced Physical Chemistry Gurdeep Raj, Goel Publishing House, Meerut
2. Physical Chemistry, P.W.Attkins,Oxford University press.
3. Physical Chemistry, R.P.Varma, Pradeep, Jalandhar
4. Physical Chemistry, G.M. Barrow, Mc GrawHill
5. Introduction to chemical thermodynamics – by R.P. Rastogi,R.R.Misra

Further Reading:

1. Quantum Chemistry,R.K.Prasad Wiley Eastren,New Delhi.
2. Quantum Chemistry by D.A.Mc Quarrie,University science books ,Mil valley, california
3. K.K.Rohatgi Mukherjee,Fundamentals of PhotoChemistry,Wiley Eastern Ltd.,1978.
4. N.J.Turro, Modern Molecular Photochemistry,Benjamin,Cumrings,Menlopark, California
5. S.Glasstone, Introduction to Electrochemistry,Affliated East West Press,New delhi
6. Principles of Physical Chemistry by Maron & Prutton

PROGRAM ELECTIVE II

SEMESTER-II

2ACPE11.1: SPECTROSCOPIC METHODS OF ANALYSIS- I

UNIT-I: UV-Visible Spectroscopy (12 Hrs)

Spectrophotometry &Colorimetry: Introduction, electromagnetic spectrum, units of wavelength, frequency and wavenumbers, the absorption laws, Absorptivity, Beer–Lambert's law Apparent deviations from Beer's law – Instrumentation –Visual comparative methods, Colorimeters, Single, Double beam spectrophotometer. Sources of radiation – Detectors —photometric accuracy, Chemical applications – Quantitative analysis –Mixture analysis– photometric titrations.

Origin and theory of UV spectroscopy, Types of electronic transitions in organic & Inorganic molecules. Chromopores, auxochromes, Applications of UV spectroscopy to simple organic molecules like conjugated dienes, trienes,unsaturated carbonyl compounds and aromatic compounds.woodward-Fieser rules.

UNIT-II: Infrared Spectroscopy and Raman Spectroscopy (12 Hrs)

Range & Nomenclature of IR, Theory of IR spectroscopy,modes of vibration, different types of vibration, Characteristic group frequencies: Alkanes, Alkenes, alkynes, cyclo alkanes and alkyl groups Aromatic compounds, alcohols, phenols ethers, cyclic ethers, amines, compounds containing carbonyl group, carboxylic acids, esters and lactones, anhydrides, nitro, nitroso and nitriles. Factors influencing vibrational frequencies, Instrumentation of IR Spectrophotometer

Raman Spectroscopy-Classical and Quantum theory of Raman effect, Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

UNIT-III: Microwave Spectroscopy&Electron Spin Resonance (12 Hrs)

Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer

Electron Spin Resonance: Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Study of free radicals.

UNIT-IV: Nuclear Magnetic Resonance Spectroscopy (12 Hrs)

Principles of Magnetic resonance, Resonance condition, Magnetic Moment & spin angular momentum, Larmor frequency, Proton Magnetic Resonance, Shielding Constants, chemical shifts, factors influencing chemical shifts, solvent shifts, Shielding & Deshielding phenomena, spin-spin coupling, coupling constants.

AX, AX_2, AX_3, AMX& AB Types of spectra, Methods of simplifying complex spectra. Double resonance technique, deuterium exchange, shift reagent, applications of PMR in structural determination-alcohols, amines, hydrogen bonding, keto-enol tautomerism, ^{19}F and ^{31}P NMR.

UNIT-V: Mass Spectrometry (12 Hrs)

Basic principles, instrumentation, Types of fragmentation, Nitrogen rule, isotope peaks, common mass fragmentation patterns of organic compounds. Fragmentation patterns of simple hydro carbons, alkyl alcohols, alkyl halides, aldehydes, ketones, aromatic compounds. Origin of meta stable ions and their uses, methods of ionization, electron ionization, chemical ionization, field ionization. Applications to inorganic systems.

Suggested books:

1. Organic Spectroscopy by W. Kemp.
2. Spectroscopy of Organic Compounds by P.S.Kalsi.
3. Spectroscopic methods in Organic Chemistry by D.H.Williams and I.Flemming.
4. Fundamentals of Molecular Spectroscopy by C.N.Banwell and E.M.Mc Cash.
5. Principles of Instrumental Analysis by Skoog and Leary.

Further Reading:

1. Optical Rotatory Dispersion: Applications to Organic Chemistryby C Djerassi.
2. NMR Spectroscopy by Harald Gunther.
3. NMR in chemistry-A multi nuclear introduction -William Kemp.
4. Spectrometric identification of organic compounds by R. M.Silverstien,G.C.Bassler and T.B.Morril.
5. Spectro metric identification of organic compounds by R.M. Silverstein and F.X. Webster.
6. Mass Spectrometry, Principles and Applications by I.Howe, D.H.Williams and R.D.Bowen,.

SEMESTER-II

PROGRAM ELECTIVE II

2ACPE11.2: BIOPOLYMER CHEMISTRY

UNIT 1: Bioenergetics and physical properties of biopolymers (12 hrs)

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement. Viscometry: Molecular weights. The Sverdberg equation.Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.

Electrophoresis : principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

UNIT II: Biological membranes (12 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport. Sodium-Potassium pump. Selective ion transport and membrane potential. The Goldman equation(derivation not required). Nerve cells.

UNIT III: binding of ligands by biopolymers (12 hrs)

Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H+ and CO_2 . Bohr effect.

UNIT IV: DNA, genes and cloning (12 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method.

Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes. Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

UNIT V: Bioinformatics (12 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment. General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB -Organism Specific Databases examples - E. Coli, Yeast, Oryza. Introduction to Proteins - primary, secondary, tertiary and quaternary structures. Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Suggested Books:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan

SEMESTER-II

OPEN ELECTIVE II

2ACOE12.1: PRINCIPLES OF CHEMICAL ENGINEERING

UNIT- I: Process calculation & Thermodynamics: (12 Hrs)

Chemical Engineering Concepts: Units and dimensions, Stoichiometric principles, Law of Conservation of Mass, Material Balance with and without chemical reactions. Laws of thermodynamics, equilibrium, phase rule.

UNIT-II: Fluid Mechanics &Particle Technology: (12 Hrs)

Fluid flow: Newton's law of viscosity, classification of fluids, Hydrostatic Pressure, Manometers, Continuity equation. Bernoulli's equation and its application, measurement of flowing fluids using orifice meter, Venturi meter and Rota meter.

Size reduction: Laws of crushing, various types of crushers and grinders-Particle terminal velocity fluidizer filtration concepts.

UNIT-III: Heat Transfer (12 Hrs)

Steady state heat transfer-Fourier's law, modes of heat transfer, simple numerical problems on conduction, natural and forced convection, heat transfer equipment, types of heat exchangers, evaporators, radiation.

UNIT-IV: Mass Transfer (12 Hrs)

Classification of mass transfer operations, choice of separation method, molecular diffusion, estimation of diffusivity of gases and liquids, Distillation: Raoult's law, vapor-liquid equilibria, relative volatility, distillation methods, azeotropic distillation. Basic principles of absorption, adsorption, extraction (qualitatively)

UNIT-V: Chemical Reaction Engineering (12 Hrs)

Overview reaction of chemical reaction engineering, classification of reactions, variables affecting the rate of reaction, definition of reaction rate, concentration dependent term of rate equation, Temperature dependent term of rate equation, Theories of Reaction rates, kinetics of homogeneous reactions, types of reactors -Classification of reactors. Catalysis: Classification preparation of catalysts, methods of characterization and evaluation of catalysts.

Suggested Books:-

1. W.C.Mccabe and J.C.Smith and peter Harriott, Unit operations of Chemical Engineering.
2. Introduction to Chemical Engineering by Ghoshal & Sanyal,Tata Mc-Graw Hill
3. Levenspiel, O.,"Chemical Reaction Eng " 3rd ed. John Wiley & sons 2001.
4. W.L.Badger and Banchero, Introduction to Chemical Engineering, Mc Graw Hill Book Co. Inc Kogakusha ,1988.

SEMESTER-II

OPEN ELECTIVE II

2ACOE12.2: PHYSICAL- ORGANIC CHEMISTRY

UNIT-I: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity(12 Hrs)

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiempirical methods and ab into and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels. Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions.
Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy.
Arrhenius equation, transition state theory. Uses of activation parameters, Hammonds postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and Selectivity principles

UNIT-II: Kinetic, isotopic, structural effects (12 Hrs)
Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects.
interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1,σR scales.

UNIT-III: solvent, steric and conformational effects (12 Hrs)
Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

UNIT-IV: Nucleophilic,electrophilic and free radical reactivity (12 Hrs)

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugality. The α-effect. - Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronsted catalysis. . nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nucleophilicity and SN2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity.

Radical and pericyclic reactivity. (a) Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and peri selectivity in pericyclic reactions.

UNIT-V: Supramolecular chemistry (12 Hrs)

Properties of covalent bonds- bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextrins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Suggested books:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH,Weinhein.
5. Physical Organic chemistry, N.S.Isaaçs

SEMESTER-II

LABORATORY III

2ACL013: ORGANIC CHEMISTRY LAB-I

Qualitative analysis of given organic compound

1. Hydrocarbons, Nitro and Halo compounds
2. Carbohydrates
3. Phenols
4. Amines
5. Carbonyl compounds
6. Acids
7. Esters

Synthesis of Organic molecules

1. Benzoin
2. M-dinitro Benzene.
3. 4-methyl umbellipherone
4. 2-phenyl indole.
5. Anthracene-Maleic anhydride adduct

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel.
2. Unitized experiments in organic chemistry by R Q Brewster.

SEMESTER-II

LABORATORY IV

2ACL14: PHYSICAL CHEMISTRY LAB-II

1. Determination of Density of unknown liquid
2. Determination of Viscosity of unknown liquid
3. Determination of Surface tension of unknown liquid

Spectrophotometry

1. Composition and stability constants of complex ions
2. Verification of Beer's Law for $Kmno_4$ and $CuSo_4$ solutions
3. Estimation of Cu (II) using EDTA
4. Estimation of Fe (III) using thiocyanate
5. Estimation of Fe (II) using 1,10-phenanthroline
6. Estimation of Fe (III) in tap water using thiocyanate by standard addition method
7. Simultaneous determination of dichromate and permanganate in a mixture

Polarimetry:

1) Determination of specific rotation of glucose and fructose
2) Enzyme catalyzed inversion of sucrose

Adsorption and others:

1. Adsorption of acetic acid on charcoal or silica gel
2. Determination of critical solution temperature of phenol-water system

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Suggested Books:

1. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical Physical Chemistry: Dr.M. Satish kumar, Sankalp Publications
5. Advanced Practical Physical chemistry: J.B.Yadav

SEMESTER III

PROGRAM CORE VII

3ACPC16: Quality Management and Intellectual Property Rights

UNIT-I Principles & Terminology in Quality Assurance: (12 Hrs)

Principles & Terminology: standard-Primary standard; standard solution, Calibration standard, check standard, *Blank:* Reagent blank, Method blank, Calibration blank, Instrumental blank, Process blank, Field blank, Equipment blank.

Calibration: Internal standardization, external standardization, addition method, control sample, dry weight, Duplicate, Duplicate samples, replicate weight.

Sampling: Basics of Sampling, Purpose of sampling ,homogeneous and heterogeneous samples, statistical criteria for good sampling ,sample size, sampling unit, gross sample, laboratory sample, Types of Samples, Representative Sample, Selective Sample, Random Sample, Composite Sample, The Sampling Plan, Legal and Statutory Requirements, Types of Sampling, Sample Numbers and Sample Size, Sampling Uncertainty, Number of Primary Samples, Sub-sampling, Sub-sampling Procedures, Sample Handling and Storage, Holding Time.

UNIT-II Quality Assurance –I (12 Hrs)

Quality control: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blind samples in quality control, use of proficiency evaluations in quality control, Analysis of standard reference materials, Analysis of duplicates.

Analytical Methods:Characteristics of an analysis, Choosing the methods – standard methods, official methods, literature methods analytical method development, Comparison of analytical methods, writing analytical methods, modification of analytical methods, Validation of new methods–ICH guidelines for method validation–sensitivity, specificity, selectivity, accuracy, precision, robustness, ruggedness, limit of detection and limit of quantitation.
, ruggedness testing of methods, 'Sign-off' and Documentation

UNIT – III Quality Assurance –II (12 Hrs)

Documentation for quality assurance.: Documentation, Quality Manual, Supporting Documentation, Record Management, Records, Generating Records, Record Identification, Document and Record Control, Reporting Results, Copying Records, Storing and Archiving Records.
General Reagents and volumetric reagents, sample labeling, sample log-in/register, sample analysis, reporting, recording and personal training. Instrument calibration and maintenance. Analytical report. Personal, training, records-professional, personnel, technician personnel. Filing quality assurance documentation.

UNIT-IV Quality Accreditation (12 Hrs)

Need for laboratory accreditation. International aspects of laboratory accreditation and in India, Criteria for laboratory accreditation, Benefits of laboratory accreditation, The Management System, The Benefits of a Management System, Types of Management Standards for Laboratories, Standards Available for Laboratories, Features of ISO 9001:2008, Features of ISO/IEC 17025:2005, Features of ISO 15189:2003. Significance of ISO 9001, 9002, 9003, 9004, Requirements, ISO/IEC 17025 Requirements, ISO 9001 Requirements, Quality Manual and other Documentation

UNIT-V Intellectual Property Rights (12 Hrs)

Definition, scope and different forms of IPR, IP laws in INDIA. International Regime of I.P.R.Procedural Aspects of Intellectual Property Rights. Patents, definition, types, contents of patent, Inventions-patentable and Non patentable, claims and types of claims, requirements for patenting, restrictions and the power of patents. Copy Rights, Trademarks and Geo Graphical Indications of goods.Plant varieties and farmer's rights, IPR Licensing and technology transfer

Suggested books:

1. Principles of instrumental Analysis – Sixth edition-skoog, Hooller, Nieman
2. Analytical chemistry – Gary D.Christian, Sixth edition, John Wiley and sons. Inc, New York 1994.
3. Quality Assurance in Analytical Chemistry, B.W.Wenclawaik, Springer, India, 2004.
4. What everyone should know about patents by N.Subbaram – Pharma Book Syndicate
5. Principles of Analytical chemistry – M.Valcarcel.

Further Reading

1. R.A Day A.C Underwood Qualitative analysis
2. Handbook of Quality Assurance for the analytical chemistry laboratory, James.P.Dux, Van
3. Nostrand Reinhood, New York, 1986.
4. Training Manuals on ISO 9000 PQM, Giridhar, Raj Publishing House, 2001
5. How to Practice GLP,PP Sharma ,vandana Publictions ,2000,New Delhi.
6. Applying ISO-9000 Quality Management systems, International Trade Centre
7. publishing,UNCTAD/WTO.Geneva,Switzerland,Indian Edition Printed by D.L.Shah Trust

SEMESTER-III

PROGRAM CORE VIII

3ACPC17: SEPARATION METHODS

UNIT-I Solvent extraction: (12 Hrs)

Principles and processes of solvent extraction, Distribution Law and Partition coefficient Nature of Partition forces, different types of Solvent extraction systems-Batch extraction, Continuous extraction, Counter current extraction, solvent extraction systems, applications in metallurgy, general applications in analysis and pre-concentration, special extraction systems like crown ethers, Super fluid and surfactant extractions-examples. Organic reagents as extraction reagents – acetylacetone, thionyl trifluoro acetone, tri-n-octyl phosphine oxide.

UNIT-II Liquid-Liquid partition Chromatography: (12 Hrs)

Principle supports, partitioning liquids, eluents, reverse phase chromatography, apparatus, and applications.

Flash Chromatography

Packing of column, selection of solvent, loading of sample.

Dry column flash chromatography - Packing of column, selection of solvent, loading of sample Medium pressure liquid chromatography (MPLC) – Apparatus, packing of column, selection of solvent, loading of sample

UNIT III Size Exclusion Chromatography: (12 Hrs)

Principles of gel – filtration Chromatography.

Instrumentation, retention behavior, resolution, selection of gel type, applications, structure of zeolite crystals, applications. Ion exclusion – principle and applications.

Capillary electrophoresis: principle, details of the instrument, Applications to Inorganic and Organic compounds.

UNIT-IV Ion -exchange chromatography (12 Hrs)

Ion -exchange resins, structure of resins. Ion exchange equilibria, selectivity, ion exchange chromatography with reference to anions and cations, applications separation of rare earth metal ions, Amino acid analysis, purification of water for laboratory and industrial use, deionized water.

Inorganic molecular sieves:structure of Zeolites,crystals,types of sieves,applicationin the separation of gases including hydrocarbons,ion exclusion- principles and applications,

Counter current chromatography- principles and application, **Affinity chromatography**- principles and applications.

UNIT-V Other methods of separation (12 Hrs)

Supercritical Fluid Chromatography (SFC)

Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Applications, technique and applications of SFC.

Membrane separations: Reverse osmosis for water purification, electro dialysis, electro-membrane processing, liquid membranes. Flotation techniques: Froth flotation, Ion flotation. Molecular sieves, clathrates.

Suggested books:

1. Separation methods by M.N. Sastri, Himalaya Publishing Company, Mumbai.
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman.
3. R.P.W. Scott, Techniques and practice of chromatography, MareldekkerInc., New York.
4. Analytical Chromatography by Gurdeep R Chatwal
5. Analytical chemistry by Gary D. Christian

Further Reading

1. Vogal Textbook of Quantitative inorganic Analysis.
2. H.M.Mc Nair and J.M. Miller, Basic Gas Chromatography, JohnWiley, New York.
3. E.Helfman, Chromatography, Van Nostrand, Reinhoid, New York.
4. Chemical separation methods,John A Dean,Von Nostrand Reinhold, New York.
5. J.A Dem Separation methods

SEMESTER-III

PROGRAM CORE IX

3ACPC18: SPECTROSCOPIC METHODS OF ANALYSIS II

UNIT-I: UV and visible spectroscopy (12 Hrs)

UV and visible spectroscopy

Quantitative aspects of absorption measurements-Beer Lamberts law, limitations of Beer's law, Numerical problems based on Beer's law, simultaneous spectrophotometer. Shapes of UV-absorption curves, solvent effects on UV-absorption bands, Instrumentation, radiation sources, Mono chromators, Detectors, Recording of the spectra, Applications in Qualitative& Quantitative analysis. Applications in transition metal complexes – Types of transition metal complexes, d-d LMCT and MLCT transitions. Band widths and shapes-nature of electronic transitions – electronic spectra-Band widths and shapes. Factors affecting Band widths.

UNIT-II: IR and Raman Spectroscopy (12 Hrs)

Infrared Spectroscopy:

Instrumentation, radiation sources, monochromators, sample cells, detectors, single beam and double beam spectrophotometer, position and intensity of the bands, finger print region, applications of IR spectroscopy for structure analysis of organic, inorganic molecules & metal chelates. Attenuated total reflectance, Nondispersive IR, applications to quantitative analysis, Quantitative analysis of multi-component mixtures. Principles of Fourier transform infrared spectroscopy and its advantages.

Raman Spectroscopy:

Theory, Instrumentation, Characteristics of Raman lines, difference between IR and Raman, applications to organic and inorganic compounds and applications in quantitative analysis.

UNIT-III NMR: (12 Hrs)

Advanced NMR Techniques: Chemical Equivalence, magnetic equivalence, double resonance decoupling, Nuclear Over Hauser Effect (NOE), Qualitative Treatment & its use, factors influencing NMR spectra, FT NMR, double resonance, spin tickling, shift reagents, applications. Continuous wave NMR. Fourier transform NMR-Basic treatment, their differences and its advantages. Two-dimensional NMR, Basic Principles, Types of 2D NMR, advantages of 2D NMR. Characteristics Nuclear properties of ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR reference standards, ranges of chemical shifts, Homo & Hetero Nuclear coupling, Structural determination of simple Inorganic compounds containing these nuclei.

UNIT-IV Mass spectrometry: (12 Hrs)

Principles. Instrumentation, Methods of ionization, field desorption, Electrospray, Atmospheric pressure, Chemical ionization, Matrix-Assisted Laser Desorption Ionization, Fast atom bombardment. Mass analyzers-magnetic sector analyzers, Quadrupole analyzers, Ion trap analyzers. Metastable ions – The origin of Metastable ions and usefulness of Metastable ions. Applications to inorganic systems: Isotopic abundance patterns for Cl, Ge, Br, Mo, Re, ReBr, ReBr2 applications in organ metallic carbonyls of $Re_2Cl_2(Co)_8$, $ReBr(Co)_5$.

Quantitative mass spectrometry: Introduction, principle, calibration and internal standards**,** general fragmentation modes of organo transition metal alkyls, carbonyls, carbonyl halides.

UNIT-V Photo Electron Spectroscopy and Fluorimetry Principles, Types (12 Hrs)

X ray photoelectron spectroscopy: Binding energies, chemical shift, structural factors on chemical shift, applications in qualitative analysis. X ray Fluorescence: principle, instrumentation, Qualitative &Quantitative applications. UV photoelectron spectroscopy of simple molecules like N_2, O_2, F_2 factors effecting UVPES.

Fluorometry: Fluorescence and chemical structure, basic principles of Instrumentation, Factors influencing intensity of Fluorescence, Fluorometric reagents, Quantitative analysis, advantages and limitations. Phosphorimetry – Theory, Instrumentation, chemiluminescence photoluminescence, applications.

Suggested books:

1. Principles of Instrumental Analysis – 5th edition – Skoog. Holler. Nieman
2. Instrumental methods of Analysis_Chatwal Anand.
3. Instrumental methodology, chemical analysis – Ewing
4. Analytical chemistry, Skoog & West
5. Hand book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle

Further Reading

1. Mass Spectrometry for Chemists and Bio-Chemists,Robert A.W.Johnstone and Malcolm.E.Rose,2nd Edition.
2. Chemical Analysis A.K. Srivatsava& Jain
3. Analytical chemistry, Gary D.Christian, Sixth edition, John Wiley and Sons. New York,
4. Instrumental methods of Analysis-B.K.Sharma,Goel Publishing House,Meerut.
5. Mass Spectrometry Principles & Applications, Hoffman & Stroobant,(Wiley)
6. Analytical NMR Ed.Ld.Field and S.Stern hill, John Wiley and Sons. New York
7. Inorganic electronic spectroscopy. A.B.P. Lever.

SEMESTER-III

PROGRAM ELECTIVE-III

3ACPE19.1: HYPHENATED AND OTHER ANALYTICAL TECHNIQUES

UNIT-I: GC-MS –Introduction (12 Hrs)

Instrumentation–GC-GC-MS interface-Mass spectrometer (MS), Instrument operation, processing GC-MS data –Ion chromatogram, Library Searching-Quantitative measurement – sample preparation, selected ion monitoring-Application of GC-MS for Trace constituents. Drugs analysis, environmental analysis and others.

Gas Chromatography-Fourier Transform-Infrared (GC-FT-IR):

Principle, Instrumentation, Applications.

UNIT-II: LC-MS –Introduction (12 Hrs)

Instrumentation –liquid chromatography- Mass spectrometer, Interface- Instrumental detailsprocessing LC-MS data –Ion chromatograms,Library Searching-Quantitative measurements.sample preparation, Selected ion monitoring-Application of LC-MS for Drugs analysis, Environmentalsamples and others.

Inductively Coupled Plasma _Mass Spectrometry (ICP-MS):

Principle, Instrumentation, Applications.

UNIT-III: Radio Chemical Methods: (12 Hrs)

Radioactive decay,Types of radiation, units and detection and measurements of radioactivity,activation analysis, isotope dilution method,tracer techniques, Radiometric titrations, Radio immuno assay.

UNIT-IV: Thermal Methods of Analysis: (12 Hrs)

a) Thermogravimetry-Theory, Instrumentation, applications with special reference to $CuSO_4.5H_2O$,CaC_2O_4 $.2H_2O$. Applications of TG study of oxalates and chromates.

b) Differential thermal analysis- Principle, Instrumentation, applications with special reference to the Clays, minerals& Coals (fuels).

c) Differential Scanning Calorimetry- Principle, Instrumentation, applications to inorganic materials like chlorates and per chlorates, ammonium nitrate. Organic Compounds and Drugs.

UNIT-V: Surface Analysis Methods (12 Hrs)

Introduction, types of surface measurements.

Photon Probe Techniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.

Suggested books:

1. Analytical Chemistry- J.G.Dick
2. Electroanalytical techniques – Kaur
3. Principles of Instrumental analysis,Skoog Holler and Neimann West, 6th edition.
4. Vogels text book of Quantitative Inorganic Analysis. Ed. Bassett et al. longmann, ELBS 3rd edition.
5. Instrumental methodology chemical analysis. Ewing.

Further Reading

1. Quntitative analysis VI Edition R.A. DayJr&AL. Underwood Prentice- Hall India.
2. Analytical chemistry, Gary D. Christian, 6th edition John Wiley and sons. Inc, New York.
3. polarographic methods in analytical chemistry M.G. Arrora
4. Instrumental methodology chemical analysis. Ewing.
5. Introduction to Inductively coupled plasma emission spectroscopy, G.I Moore, Elsevier Science Publisher, New York
6. Applications of ICP-MS, A.R. Date and A.L. Glay, London (Eds), Blakie, London
7. Instrumental techniques for Analytical chemistry, Ed. Frank Settle.

SEMESTER-III

PROGRAM ELECTIVE-III

3ACPC19.2: MEDICINAL INORGANIC CHEMISTRY

UNIT-I: Metal complexes as Drugs and Anticancer agents (12 Hrs)

Introduction to Pt (II) chemistry – Thermodynamic and kinetic principles – Cis and Trans influences – Thermodynamic and kinetic aspects.

Platinum complexes in cancer therapy: Discovery applications and structure-effect Relationships. Cis platin(cis Pt (NH3)2Cl2) mode of action. Drug resistance and DNA repair mechanism. Physical effects of metal complex: DNA binding, unwinding, shortening and bending of the double helix. Biological consequences of platinum –DNA binding. Organic intercalators as donor – acceptor pairs; Transition metal complexes as donor acceptor pairs. Non classical platinum antitumor agents.

UNIT-II: Metal complexes in Clinical Chemistry (12 Hrs)

Theory and mode of action of therapeutic chelating agents, Single ligand Chelation Therapy – Aminopolycarboxylic acids, Desferrioxamine, pencillamine, triethylenetetramine, Mixed ligand chelation therapy - Metallothionens in detoxification. Role of metal ions in the action of antibiotics: Bleomycin, Adriamycin and tetracyclines. Gold-Containing drugs used in therapy of Rheumatoid arthritis - A therapeutic agent for Menkes disease: Copper-histidine - Anti viral chemotherapy and metal peptide interaction.

UNIT-III: Chemical probing of DNA complexes (12 Hrs)

Chemical probing of DNA complexes: Introduction to foot printing. Chemical probing. Attack on DNA bases a) dimethyl sulfate b) diethyl pyro carbonate c) osmium tetroxide d) ldehydese) ethyl nitrosourea (ENA) and other chemical probes like tris phenanthroline metal complexes.

UNIT-IV: Photochemical probing of DNA complexes (12 Hrs)

Photochemical probes: Psoralens, acridines, UV radiation Enzymatic probes Immobilization of enzymes: Methods and Applications. Platinum Metal Complexes as drugs and anticancer agents: Importance of binding and photoreactive metal complexes, ligand dissociation and photoactive metal complexes, ligand dissociation and photo substitution, photo physics and photochemistry of Ru (II) polypyridyl complexes. Photo physics and photochemistry of Ru(ii) polypyridyl complexes. Photo physics in the absence of DNA and in the presence of DNA.

UNIT-V: DNA binding and molecular pharmacology and Interaction of Metallo (12 Hrs)

Pharmaceuticals

Introduction, concept of intercalating a) classical model b) developments of intercalation model c) quantitative analysis of intercalation.

Factors which relate intercalation and medicinal activity a) Binding constant b) kinetics c)structural effects and activities d) intercalation and drug action Specific drugs which bind to DNA by intercalation: a) antipyranosomal drugs b) antimalarial drugs c) antitumor drugs.

Nonspecific interaction in dye binding to DNA and influence of alcohols and amides.

Ruthenium: Ru (III), amine complexes: Antitumor activity, structure activity relationship DNA binding and cleavage - DMSO complexes of Ru (II): DNA interactions of polyaromatic amines - Ru (IV) complexes oxidative DNA cleavage. Rhodium: Rhodium (II) acetate dimer. Anticancer

activity metallocene, Chemical correlation with antitumor activity, DNA binding and mechanistic possibility. Introduction, Structural and chemical properties of streptogramin and its metal complexes - Evidence for formation of ternary complexes involving DNA and its components. Antitumor activity and mechanism - Metal induced free radical production by organic drugs in relation to their side effects.

Suggested Books

1. Bioinorganic Chemistry. Inorganic elements in the Chemistry of life, Wolfgang Kaim & Brigette Schwederdki.
2. Handbook of Metal-Ligand interactions in Biological fluid Bioinorganic medicine, Vol – 2 : Edt. Guy Berthon.
3. Bioinorganic Chemistry, Rosette M. Roat Malone.
4. Photoreactions of Metal complexes with DNA, A. Krisch – De Mesmacker et al.

SEMESTER-III

OPEN ELECTIVE-III

3ACOE20.1: FOOD TECHNOLOGY, PHARMACEUTICAL & ENVIRONMENTAL ANALYSIS

UNIT I (12 Hrs)

Analysis of Food, Additives and Pesticide residues

Analysis of Food:

Determination of starch by saccharimetric method in flour. Analysis of dairy products, Analysis of caffeine in Tea and Coffee Analysis of chemical additives: Division of color additives (Coal – tar dyes, vegetable colors and mineral colors) chromatographic identification of colors, quantitative estimation of added dyes in foods.

Analysis of Food Additives: Chemical preservatives and synthetic sweetening agents (organic – ether extractable and non-ether extractable) SO_2, Sodium Benzoate, Sorbic acid, Benzoic acid. Antioxidants: Types of Antioxidants used in foods, analysis of butylated hydroxy toluene (BHT) by TLC & GC.

Analysis of Pesticide residues: Analysis of pesticide residues Endosulfan, endrin, BHC,2,4-D,2,4,5-T by HPLC.

UNIT II Preformulation (12 Hrs)

Goals of Preformulation, solid state manipulation and characterization. pH dependent solubility of drug, equilibrium solubility, intrinsic dissolution of drug, particle size distribution.
Flow of Powders: Physical properties and importance. Angle of repose, Cars index, compressibility, bulk density, tapped density

UNIT III Process quality control tests (12 Hrs)

In process quality control tests for Oral solid dosages forms (Tablets, capsules etc.,) and parenteral (Injection etc.,)

Hard Gelatin Capsules: General principles and steps involved in the production of drug loaded hard gelatin capsules, filling operation, filling of powders, granules and pellets.

Tablets: Types of tablets, granulation methods, highlighting operations such as mixing, drying, milling, blending, lubrication and compression, disintegration, dissolution.

Unit IV: Stability testing (12 Hrs)

Chemical degradation and preventive measures. Various stability testing conditions and use of stabilizers in packing

UNIT-V: Analysis of Air, water and solid wastes (12 Hrs)

a) Analysis of Air:

Air pollutants, Chemical analysis of Air pollutants

Primary air pollutants: Carbon compounds ($CO\&CO_2$)
Sulphur compounds (SO_2, $SO_3\&H_2S$)

Nitrogen compounds ($NO\&NO_2$)
Hydrocarbons(Aliphatic hydrocarbons, Polycyclic
Aromatic hydrocarbons)
Secondary air pollutants: Ozone, Peroxy Acetyl Nitrate(PAN)
b) Analysis of water: Analytical methods for analysis of following ions, Determination pH and TDS
Anions:carbonate, bicarbonate, fluorine, chlorine, Bromine and Iodine, sulphate, phosphate, nitrate, cyanide.
Cations: Na, K**,** Fe-(II), Fe-(III), Ca-(II), Mg-(II), Cr-(III), Cr-(VI)

c) Analysis of solid wastes, soils: Sampling, determination of moisture, soil adsorption ratio. Analysis of environmental samples (soil and solid wastes for inorganic and organic pollutants): volatile and semi volatile hydrocarbons, Poly Aromatic Hydrocarbons (PAHs) and chlorinated pesticides and inorganic cations and anions utilizing appropriate separation methods followed by analysis using GC and HPLC

Suggested books:

1. Environmental Pollution Analysis – S.M.Khopkar, Wiley Eastern Limited
2. Environmental Chemistry –B.K.Sharma – H.Kaur
3. Pharmaceutical chemistry, Instrumental techniques Vol-2, Edited by Leslie.G.Chatten.
4. Text Book of Pharmaceutical analysis – Kenneth. A.Connors
5. Handbook of analytical control of Iron and steel production,Harrison John, wiley 1979.

Further Reading

1. Technical Methods of Analysis,Griffin,Mc GRaw Hill
2. Environmetal Analysis – Chatwal
3. Environmental Analysis – C.S.Rao or S.M. khopkar(IIT Bombay)
4. A text book of Environmental Control & Pollution – S.S.Dara.
5. Handbook of analysis and quality control for fruit and vegetables products- S.Ranganna.
6. Practical pharmaceutical chemistry, A.H.Beckett and J.B.Stenlake, III edition Vol &Vol.2.
7. 17. Hand Book in Analysis and quality control for fruit and vegetable products-S.Ranganna.

SEMESTER-III

OPEN ELECTIVE-III

3ACOE20.2: LABORATORY ANALYSIS AND MANAGMENT

UNIT-I: (12 Hrs)

Practical Aspects of Chemical Analysis: Analysis of real samples - Choice of analytical method; Literature survey; Analysis of standard samples; Preparing samples for analysis – preparing laboratory samples; moisture in samples; drying the analytical sample; decomposition and dissolution of sample and source of errors in decomposition and dissolution

UNIT-II: Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) -Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications

Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle, Instrumentation, applications. Atomic Force Microscopy - Principle, Instrumentation, applications.

UNIT-III: Micromeritics, Dissolution and disintegration (12 Hrs)

Particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method). Dissolution: Drug absorption, theories of drug dissolution – Diffusion layer model, Danckwert's model & interfacial barrier model. Dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus). Disintegration tests for tablets, capsules and enteric coated tablets.

UNIT-IV: Automation in Laboratory (12 Hrs)

Introduction, classification of Analytical methods, Types of Instrumental methods, Instruments for analysis. Analog & Digital signals, Planning for laboratory automation. An overview of automatic instruments & instrumentation. Flow Injection Analysis, Discrete automatic systems.

Good laboratory practices: Instrumental standardization, optimization of procedures.

UNIT-V: LIMS and Computer aided Analysis (12 Hrs)

Laboratory Information Management System: Laboratories as information producers, properties of good information, Laboratory information management system, conclusions.

Computer aided analysis: Computer-instrument interaction, computer organization- Hardware - Basic Digital circuit components, Microprocessors and Microcomputers, Computer Software - Software control of the computer-instrument interfaces. Automated laboratory – Automated instruments (AAS), Applications of computers, Computer Networks.

Suggested Books

1. Structural methods in Inorganic Chemistry - E.A.V. Ebsworth, et al., ELBS Publications, 1988.
2. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-Hill Publishing Company Ltd
3. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York,

4. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed. Blackwell Science, 2000.
5. Instrumental Methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.

Further reading

1. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork,2003.
2. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.

SEMESTER-III

LABORATORY-V

3ACL21: WET ANALYSIS LAB

Titrimetry

1. Determination of Ca2+, Mg2+, CO3 2- & HCO3 - in soil sample.
2. Determination of Fe & Ca in Cement
3. Determination of Saponification value and Iodine value of an oil sample
4. Determination of Ampicillin and amoxicillin
5. Determination of Ampicillin and Di cloxacillin in combined form
6. Analysis of Albendazole drug by Non-Aqueous Titrations
7. Analysis of Atenolol drug by Non-Aqueous Titrations
8. Analysis of Glipizide drug by Non-Aqueous Titrations
9. Analysis of Domperidone drug by Non-Aqueous Titrations
10. Analysis of chloro pheneramine maleate drug by Non-Aqueous Titrations

SEMESTER-III

LABORATORY-VI

3ACL22: ANALYTICAL INSTRUMENTION LAB

Spectroscopic and chromatographic methods of analysis of drugs and pharmaceuticals

a) Identification and Estimation using UV - Vis Spectrophotometer

1. Estimation of Paracetamol
2. Estimation of Ampicillin
3. Estimation of ciprofloxacin
4. Estimation of Domperidone
5. Estimation of Metformin
6. Estimation of Oxyclozanide
7. Estimation of Doxycycline
8. Estimation of Cefuroxime axetil
9. Estimation of Gliclazide

b) Chromatography

1. HPLC study of two available drugs. Ex
2. GC study of two available drugs.

c) Synthesis of organic compounds, their identification and estimation (TLC, IR, UV Vis Spectrophotometer) 2 Examples

Suggested books:

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R. Hememan etal John Wiley & Sons 1984.
2. Analytical Chemistry by Gary D.Christian 6th Edition John Wiley & Sons Inc New York 1994.
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson EducationLtd 2002.
4. Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors1994.
5. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. 1996