

COURSE STRUCTURE AND SYLLABUS
M.Sc (Analytical Chemistry)
CHOICE BASED CREDIT SYSTEM (CBCS)



(With effect from 2019-2020 onwards)

CENTRE FOR CHEMICAL SCIENCES AND TECHNOLOGY
INSTITUTE OF SCIENCE & TECHNOLOGY
(Autonomous)
JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY
HYDERABAD
KUKATPALLY, HYDERABAD.-500085, TELANGANA
CENTRE FOR

CHEMICAL SCIENCES & TECHNOLOGY (CCST)
M.Sc ANALYTICAL CHEMISTRY
COURSE STRUCTURE
(W.E.F-2019-20 BATCH)

I YEAR

I semester		Course Title	Int. Marks	Ext. marks	L	P	C
1.	Core Course I	Organic Chemistry – I	25	75	4	-	4
2.	Core Course II	Inorganic Chemistry	25	75	4	-	4
3.	Core Course III	Physical Chemistry-I	25	75	4	-	4
4.	Core Elective I	(i) Principles of Analytical Chemistry (ii) Bio Molecules	25	75	4	-	4
5.	Open Elective I	(i) Applied Chemistry (ii) Computers and mathematics	25	75	4	-	4
6.	Laboratory I	Inorganic Chemistry Lab	25	50	-	6	3
7.	Laboratory II	Physical Chemistry Lab-I	25	50	-	6	3
Total			175	475	20	12	26

II semester		Course Title	Int. Marks	Ext. Marks	L	P	C
1.	Core Course IV	Organic Chemistry – II	25	75	4	-	4
2.	Core Course V	Instrumental Methods of Analysis	25	75	4	-	4
3.	Core Course VI	Physical Chemistry-II	25	75	4	-	4
4.	Core Elective II	(i) Spectroscopy and spectrometry (ii) Applied Analysis	25	75	4	-	4
5.	Open Elective II	(i) principles of chemical engineering (ii) Physical Organic Chemistry	25	75	4	-	4
6.	Laboratory III	organic Chemistry Lab –I	25	50	-	6	3
7.	Laboratory IV	Physical Chemistry Lab-II	25	50	-	6	3
		SEMINAR	---	50	--	3	2
Total			175	525	20	15	28

II YEAR

III semester		Course Title	Int. Marks	Ext. Marks	L	P	C
1.	Core Course VII	Quality Management and IPR	25	75	4	-	4
2.	Core Course VIII	Separation Methods	25	75	4	-	4
3.	Core Course IX	Spectroscopic Methods Of Analysis	25	75	4	-	4
4.	Core Elective III	(i) Hyphenated & Other Analytical Techniques (ii) Medicinal Inorganic Chemistry	25	75	4	-	4
5.	Open Elective III	(i) Food Technology, Pharmaceutical & Environmental Analysis (ii) Laboratory Analysis and	25	75	4	-	4
6.	Laboratory V	Wet Analysis Lab	25	50	-	6	3
7.	Laboratory VI	Analytical Instrumentation Lab	25	50	-	6	3
	Seminar		---	50	-	3	2
	Total		175	525	20	15	28

IV Semester		Int. Marks	Ext. Marks	L	P	C
1.	Comprehensive Viva -Vove	-	100	-	-	4
	Project Work Review	50	-	-	8	2
2.	Project Evaluation (VivaVove)	-	100	-	16	8
	Total	50	200		24	14

Total Marks: 650+700+700+250=2300

Total Credits: 26+28+28+14=96

SEMESTER-I

CORE COURSE –I

ACT-101: 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 with chiral centers. 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: Heterocycles 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

(12 Hrs)

Carbohydrates and vitamins: 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 A₁, B₁, B₂, B₆, 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, Sommelet - Hauser and Smiles).

Recommended 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. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J.A. Joule, K. Mills and G.F. Smith, Stanley Thornes Ltd, UK, (1998)
6. The Chemistry of Indole, R.J. Sundberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn. R.M. Acheson, Interscience Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by RT Morrison and RN Boyd.
13. Organic Chemistry, Vol. 2 by I.L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege

SEMESTER-I

CORE COURSE –II

ACT-102: 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: (12 Hrs)

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 Globin 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 Lability 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 , C_s , 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.

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) Factors favoring 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 $Re(III)$.

Recommended 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. BioInorganic Chemistry- K.Hussain Reddy
6. Selected Topics in Inorganic chemistry madan, Malik, Tuli S.Chand publications.
7. Inorganic reaction Mechanism- F.Basolo & R.G.Pearson, New York.
8. Inorganic Chemistry- Keith F.Purcell & John C.Kotz Holt- Saunde International Edition.
9. Ligational aspects of diatomic molecules-Organometallic Chemistry R.C.Mehotra.
10. Bio-inorganic Chemistry, Gopalan
11. K.V.Raman, Group Theory and its applications to Chemistry, Tata McGraw Hill Publishing Co.1990
12. Group theory by F.A.Cotton

SEMESTER-I

CORE COURSE –III

ACT – 103 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 Clausius-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)

Electrodeics:

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 Lindemann's theory. Salt effects.

Complex Reactions

Opposing reactions, parallel reactions, consecutive reactions (all first order type). Chain reactions, chain length, Rice Herzfeld 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: Michaelis-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.

Recommended 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
5. Quantum Chemistry,R.K.Prasad Wiley Eastren,New Delhi.
6. Quantum Chemistry by D.A.Mc Quarrie,University science books ,Mil valley, california
7. Solid State Chemistry, K.F.Purcell and J.C. Klotz
8. Solid State Chemistry,A.R.West,John Wiley, 1990
9. Thermodynamics by J. Rajaram, and J.C. Kuriakose
10. Fundamentals of Quantum chemistry.by R.Anatha Raman,Mcmillan India Ltd,2001.
11. P.W.Atkins,physical chemistry,Oxford University press.

SEMESTER-I

CORE ELECTIVE- I

ACT-104.1 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.

Recommended 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. Pietrzyk and Frank. Analytical chemistry, 1990.
4. KVSG Muralikrishna, An Introduction to ISO 14000, Environmental Management, 1998.
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

CORE ELECTIVE- I

ACT-104.2 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),B₆ (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- Metoprolol, 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.

Recommended books:

1. Enzyme structure and mechanism by Fersht and Freeman
2. Bio-Organic chemistry by Hennen Dugas
3. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
4. Lehninger Principles of Biochemistry by D L Nelson and M Cox
5. Outlines of Biochemistry by Conn and Stumpf
6. Biotransformations in Organic Chemistry by K Faber.
7. Principles of biochemistry by Horton & others.
8. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
9. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
10. Introduction to Medicinal chemistry. By Graham Patrick.
11. Introduction to drug design. By R.B.Silverman
12. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
13. Principles of medicinal chemistry. By William O. Foye et al.
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
15. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
16. Drug design By E.J. Arienes
17. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam et al
18. Medicinal chemistry An introduction By Gareth Thomas

SEMESTER-I

OPEN ELECTIVE- I

ACT-105.1: 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:

(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

Crystalization Techniques: 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, Cationic polymerizations. Molecular weight of polymers M_w , M_n 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.

Recommended Books:

1. A Text book of engineering chemistry –Jaya Shree Anireddy. Willey precise textbook series, Willey 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.
5. Comprehensive engineering chemistry-Devender singh, Balsaraf, Satish Kumar Vats, I.K.International.
6. Chemical process industry safety by K S N Raju, Mc Graw Hill Education, 2014
7. Nanotechnology in Catalysis by Pinzhan
8. Springer Handbook of Nanotechnology by Bharat Bhushan
9. Introduction to Polymer Chemistry by Charles E.Carraher.
10. Textbook of Polymer Chemistry by Man P Singh.
11. Organic Chemistry by Marye Anne Fox, James K. Whitesell.

SEMESTER-I

OPEN ELECTIVE- I

ACT-105.2: 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-tokens-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 Dimensionality Reduction

Recommended 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

LABORATORY-I

ACP – 106: 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) $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$,
 - g) $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Cl}_2$,
 - h) $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{Cl}_2$
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 Ferricyanide.

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

ACP – 107: PHYSICAL CHEMISTRY-LAB-I

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

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 at two different strengths and compare the relative strengths of the acid.
2. Hydrolysis constant of urea hydrochloride-ester hydrolysis method.
3. Study of saponification of ethyl acetate by NaOH and determination of rate constant.
4. Kinetics of persulphate $(S_2O_8)^{2-}$ and I⁻ reaction

Overall order

1. Order with respect to (I)
2. Order with respect to $(S_2O_8)^{2-}$
3. Effect of salt (KCl) on the rate of the reaction.
4. Effect of temperature on rate - determination of energy of activation.

Text 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

CORE COURSE IV

ACT-201: ORGANIC CHEMISTRY – II

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 diastereomers & enantiomers, factors affecting conformational stability and conformational equilibrium-attractive and repulsive interactions of cyclic systems.

Unit II: 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

Unit-III: Photochemistry

(12 Hrs)

Photo physical processes and photochemical processes. Electronically excited molecules-singlet and triplet states. Jablonski diagram. Photochemistry of carbonyl compounds - $n - \pi^*$, $\pi - \pi^*$ transitions, Norrish type I and Norrish type II cleavages, Petermann-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 IV: 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 V: Heterocyclic Compounds-II

(12 Hrs)

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

Recommended 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, Stanley Thornes Ltd, UK, (1998)
5. The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York (1970).
6. An introduction to the chemistry of heterocyclic compounds, 2nd Edn. R.M. Acheson, Interscience Publishers, New York, 1967.
7. Advanced Organic Chemistry by Jerry March
8. Mechanism and Structure in Organic Chemistry S. Mukerjee
9. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
10. Organic Chemistry by RT Morrison and RN Boyd.
11. Organic Chemistry, Vol. 2 by I.L. Finar.
12. Organic Chemistry: Structure and Reactivity by Seyhan Ege.
13. Pericyclic Reactions by Mukherjee S M
14. Conservation of Orbital Symmetry by Woodward and Hoffmann
15. Photochemistry by C W J Wells
16. Organic Photochemistry by Turro
17. Molecular Photochemistry by Gilbert & Baggo
18. Organic Photochemistry by D Coyle

SEMESTER-II

CORE COURSE V

ACT-202: INSTRUMENTAL METHODS OF ANALYSIS

UNIT-I: 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-II: 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.

UNIT-III: 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-IV: 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-V: 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.**

Recommended books:

1. R.A.Day& A.L.Underwood, Quantitative analysis, Prentice-Hall of India Pvt. Ltd., 1985.
2. Skoog & West, Fundamentals of Analytical Chemistry, 1982.
3. Hobert H. Willard, D.L.Meritt & J.R.J.A.Dean, Instrumental methods of analysis, C.B.S Publishers and Distributors, 1992.
4. Vogel, Textbook of quantitative inorganic analysis, 1990.
5. Ewing, Instrumental Methods of Analysis, 1992.
6. Instrumental Methodology of Analysis by Chatwal Anand.

SEMESTER-II

CORE COURSE VI

ACT-203: 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-singlet and 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 absorption isotherms-study of kinetics of surface reactions catalysis by metals, semiconductor oxides-mechanism of heterogeneous catalytic reactions-the absorption 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.

Recommended Books:

1. Advanced Physical Chemistry Gurdeep Raj, Goel Publishing House, Meerut
2. Introduction to chemical thermodynamics – by R.P. Rastogi,R.R.Misra
3. Chemical Kinetics by K.J.Laidler
4. Physical Chemistry, G.M. Barrow, Mc GrawHill
5. Quantum Chemistry,R.K.Prasad Wiley Eastren,New Delhi.
6. Quantum Chemistry by D.A.Mc Quarrie,University science books ,Mil valley, california
7. Solid State Chemistry, K.F.Purcell and J.C. Klotz
8. Solid State Chemistry,A.R.West,John Wiley
9. Physical Chemistry, P.W.Atkins,Oxford University press.
10. Physical Chemistry, R.P.Varma, Pradeep, Jalandhar.
11. K.K.Rohatgi Mukherjee,Fundamentals of PhotoChemistry,Wiley Eastern Ltd.,1978.
12. N.J.Turro, Modern Molecular Photochemistry,Benjamin,Cumrings,MenloPark, California
13. S.Glasstone, Introduction to Electrochemistry,Affiliated East West Press,New delhi
14. Principles of Physical Chemistry by Maron & Prutton
15. Engineering Chemistry, C.Pameswara Murthy, C.V.Agarwal and A. Naidu, B.S. Publications, Hyderabad

SEMESTER-II

CORE ELECTIVE II

ACT – 204.1: SPECTROSCOPY AND SPECTROMETRY

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. Chromophores, 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- 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, AX₂, AX₃, 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, ¹⁹F and ³¹P 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 hydrocarbons, alkyl alcohols, alkyl halides, aldehydes, ketones, aromatic compounds. Origin of metastable ions and their uses, methods of ionization, electron ionization, chemical ionization, field ionization. Applications to inorganic systems.

Recommended books:

1. W.Kemp, Organic Spectroscopy, 3rd edition, ELBS, Mc Millan, London, 1991.
2. P.S.Kalsi, Spectroscopy of Organic Compounds, 4th edition, New Age International (P) Ltd., Publishers, Hyderabad – 29.
3. D.H.Williams and I.Flemming, Spectroscopic methods in Organic Chemistry, 4th edition, Mc Graw Hill, New York, 1989.
4. C.N.Banwell and E.M.Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition Tata Mc Graw Hill, New Delhi, 1995.
5. I.Howe, D.H.Williams and R.D.Bowen, Mass Spectroscopy, Principles and Applications, 2nd edition, Mc Graw Hill, London, 1981.
6. C.Djerassi, Optical Rotatory Dispersion.
7. Harald Gunther, NMR Spectroscopy, 2nd edition, John Wiley & Sons (1996).
8. NMR in chemistry-A multi nuclear introduction -William Kemp.
9. Spectroscopic identification of organic compounds by R.M. Silverstein, G.C. Bassler and T.B. Morrill
10. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
11. Organic spectroscopy by William Kemp
12. Spectroscopic identification of organic compounds by R.M. Silverstein. G.C. Bassler and T.E. Morrill
13. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.

SEMESTER-II

CORE ELECTIVE II

ACT-204.2: APPLIED ANALYSIS

UNIT-I: Analysis of Finished Products and ores

(12 Hrs)

Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous.

Analysis of non- Ferrous alloys: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder.

Analysis of Cement: Composition of Portland cement, estimation of Aluminium oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography

Ores:

a) Iron ore- Analysis of the Constituents – Moisture, loss of ignition, Total Iron, ferrous Iron, ferric Iron, alumina, Silica, Titania, Lime, Magnesia, Sulphur, phosphorous, manganese, alkalies, combined water, Carbon in blast furnace, flue dust and sinter.

UNIT-II: Analysis of Air and Water Pollutants

(12 Hrs)

Air quality standards, sampling, analysis of air pollutants-SO₂ (UV_Vis, IR), H₂S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NO_x (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO₂ (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O₃ (Chemiluminescence & Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total dissolved solids (turbidimetry), Chemical analysis of anions – CN⁻, Cl⁻, F⁻, NO₂⁻, NO₃⁻ (spectrophotometry), SO₄, PO₄. Determination of BOD, COD, TOC & DO Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

UNIT-III: Clinical and Pharmaceutical Analysis

(12 Hrs)

Clinical Analysis: Determination of (1) Serum Calcium (2) Serum/Plasma Bicarbonate (Titrimetry). Determination of Serum Chloride (Coulometry) - Determination of (1) Cholesterol (2) Total Protein (3) Blood Urea in Serum (4) Amylase (5) Aspartate Amino Transferase (AST) and Alanine Amino Transferase (ALT) (by Spectrophotometry). Determination of (1) Thyroxin and (2) Thyroid-Stimulating Hormone (TSH) (by RIA Method)

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometric), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin, paracetamol and codeine in APC tablets (NMR), Phenobarbitone in tablets (IR), pivalic acid in dipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC_MS).

UNIT-IV: Food Analysis

(12 Hrs)

Food Analysis: Analysis of Chemical Additives in foods : Division of colour additives, Chromatographic identification of colors, and quantitative estimation of added dyes in foods (Titanium Trichloride Method) - chemical preservatives and synthetic sweetening agents

Organic-ether extractable and Non-ether extractable) - Analysis of SO₂& Sodium Benzoate (Chemical Methods), Sorbic Acid (Chromatography) - Types of Antioxidants used in Foods, Analysis of Butylated Hydroxy Toluene (BHT) (Spectrophotometry).

UNIT-V Agricultural Analysis:

(12 Hrs)

Analysis of soils for available Major Nutrients - Estimation of available Nitrogen (Kjeldahl Method), Phosphorus (Olsen's Method and Bray and Kurtz Method), and Exchangeable Calcium & Magnesium (by EDTA). Soil analysis for Micronutrients - Estimation of Available Zinc, Copper, Manganese and Iron (AAS)- Analysis of Pesticide Residues - Determination of Methyl Parathion Residues in food grains & vegetables (Solvent Extraction and Titrimetry) - Determination of Organochlorine pesticides by Gas Chromatography (Cypermethrin) - Determination of Malathion and DDT Residues in food grains (Spectrophotometry).

SUGGESTED BOOKS

1. Analytical Chemistry, Gary Christian, VI Ed, John Wiley & Sons Inc, New York.
2. Fundamentals of Analytical Chemistry, Skoog & West.
3. Pharmaceutical Drug Analysis, Ashtoshka.
4. Vogel's Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd.
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995.
6. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie Academi Professional.
7. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
8. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd, 1986.
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors.
10. Practical pharmaceutical Chemistry, a H Beckett and J B Stenlake, III Ed, Vol I and Vol II, CBS Publishers & Distributors, 1997.
11. Pharmaceutical Analysis, David G Watson, Churchill Livingstone Harcourt Brace and Company Ltd, 1999.
12. Handbook of analysis of drugs, Nagavi.
13. Medical Laboratory Technology – Mukherjee , Tata Mc Graw Ltd 1988.
14. Medical Laboratory Technology – Ramnik Sood , Jaypee Brothers Ltd 1999.
15. Text Book of Clinical Chemistry V Edn Carl.A. Burtis Edward R. Ashwood Saunders Harcourt India 2001.

SEMESTER-II

OPEN ELECTIVE II

ACT-205.1: 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.

Recommended 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 Banchemo, Introduction to Chemical Engineering, Mc Graw Hill Book Co. Inc Kogakusha, 1988.

SEMESTER-II

OPEN ELECTIVE II

ACT-205.2: 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 initio 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, σ_1, σ_R 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, calixerenes, cyclodextrins. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Recommended books:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
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, Weinheim.
5. Physical Organic chemistry, N.S.Isaaçs
6. Supramolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack Hine

SEMESTER-II

LABORATORY III

ACP-206: PHYSICAL CHEMISTRY LAB-II

Spectrophotometer

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

Recommended Books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav

SEMESTER-II

LABORATORY IV

ACP-207: ORGANIC CHEMISTRY LAB-I

Qualitative organic analysis – identification of a single substance of at least eight compounds.

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

synthesis of Organic molecules – one stage preparations of the following.

- a) Benzoin
- b) Tribromo aniline
- c) m-dinitro Benzene.
- d) 4-methyl umbelliferone
- e) 2-phenyl indole.
- f) Anthracene-Maleic anhydride adduct

SEMESTER III

CORE COURSE VII

ACT-301 Quality Management and Intellectual Property Rights

UNIT-I Principles & Terminology in QA: (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

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

SEMESTER-III

CORE COURSE VIII

ACT-302 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,application in 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.

Recommended books:

1. Separation methods by M.N. Sastri, Himalaya Publishing Company, Mumbai.
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman.
3. J.A Dem Separation methods
4. R.P.W. Scott, Techniques and practice of chromatography, MareldekkerInc., New York.
5. Analytical Chromatography by Gurdeep R Chatwal
6. Analytical chemistry by Gary D. Christian
7. Vogel Textbook of Quantitative inorganic Analysis.
8. H.M.Mc Nair and J.M. Miller, Basic Gas Chromatography, JohnWiley, New York.
9. E.Helfman, Chromatography, Van Nostrand, Reinhold, New York.
10. Chemical separation methods,John A Dean,Von Nostrand Reinhold, New York.

SEMESTER-III

CORE COURSE IX

ACT-303: SPECTROSCOPIC METHODS OF ANALYSIS

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

UV and visible spectroscopy

Quantitative aspects of absorption measurements-Beer Lambert's 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 ^1H , ^{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 organometallic carbonyls of $\text{Re}_2\text{Cl}_2(\text{CO})_8$, $\text{ReBr}(\text{CO})_5$.

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 N₂, O₂, F₂ 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.

Recommended books:

1. Principles of Instrumental Analysis – 5th edition – Skoog, Holler, Nieman
2. Hobert.H. Wittard D. L Meritt and J.K.A. Dean Instrumentation –C.B.S. Publisheres
3. Inorganic electronic spectroscopy. A.B.P. Lever.
4. Chemical Analysis A.K. Srivatsava& Jain
5. Instrumental methodology, chemical analysis – Ewing
6. Infrared and Raman spectra of Inorganic and coordination compounds, Kazuo Nakamoto, 5th edition, John Wiley & Sons, 1955.
7. Mass Spectrometry for Chemists and Bio-Chemists, Robert A.W. Johnstone and Malcolm.E.Rose, 2nd Edition.
8. Hand book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle Prentice Hall, New Jersey, USA (1997).
9. Analytical chemistry, Gary D.Christian, Sixth edition, John Wiley and Sons. New York, 1994.
10. Analytical chemistry, Skoog & West, 6th edition.
11. Instrumental methods of Analysis_ Chatwal Anand.
12. Instrumental methods of Analysis-B.K.Sharma, Goel Publishing House, Meerut.
13. Mass Spectrometry Principles & Applications, Hoffman & Stroobant, 2nd Ed.(Wiley) 20003.
14. Analytical NMR Ed.Ld.Field and S.Stern hill, John Wiley and Sons. New York, 1989.

SEMESTER-III

CORE ELECTIVE-III

ACT-304.1 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 $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. 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.

Recommended 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. W.Jeumings, Analytical gas chromatography, Academic Press, New York
6. Quantitative analysis VI Edition R.A. DayJr&AL. Underwood Prentice- Hall India.
7. Analytical chemistry, Gary D. Christian, 6th edition John Wiley and sons. Inc, New York, 1994.
8. polarographic methods in analytical chemistry M.G. Arrora
9. Instrumental methodology chemical analysis. Ewing.
10. Introduction to Inductively coupled plasma emission spectroscopy, G.I Moore, Elsevier Science Publisher, New York, 1989.
11. Applications of ICP-MS, A.R. Date and A.L. Glay, London (Eds), Blakie, London
12. Instrumental techniques for Analytical chemistry, Ed. Frank Settle.
13. R.A Day A.C Underwood Qualitative analysis.
14. Wendlandt, Thermal Analysis, John Wiley Sons, New York.

SEMESTER-III

CORE ELECTIVE-IV

ACT-304.2 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) Idehyde) 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 & Brigitte Schwederki.
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

ACT-305.1: 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) SO₂, 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, Carr's 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&CO₂)

Sulphur compounds (SO₂, SO₃&H₂S)

Nitrogen compounds (NO&NO₂)

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

Recommended 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.
6. Standar mehods of Chemical Analysis,welcher
7. Technical Methods of Analysis,Griffin,Mc GRaw Hill
8. Environmetal Analysis – Chatwal
9. Aquatic Environmental Chemistry – Alan G.Howard
10. Environmental Analysis – C.S.Rao or S.M. khopkar(IIT Bombay)
11. A text book of Environmental Control & Pollution – S.S.Dara.
12. Biochemical methods – 2nd edition. S.Sadasivan, A.Manickam
13. Handbook of analysis and quality control for fruit and vegetables products- S.Ranganna.
14. Practical pharmaceutical chemistry, A.H.Beckett and J.B.Stenlake, III edition Vol 1 & Vol.2.
15. Pharmaceutical analysis. P.Parimoo.
16. Environmental Chemistry – 4th edition – Anil Kumar.De Wiley Eastern Ltd.
17. Hand Book in Analysis and quality control for fruit and vegetable products-S.Ranganna.

SEMESTER-III

OPEN ELECTIVE-III

ACT-305.2: 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. Physical Methods in Chemistry - R.S. Drago, W.B. Saunders Co, 1977.

3. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-Hill Publishing Company Ltd., 1985.
4. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York, 1994.
5. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998
6. Principles and practice of Analytical Chemistry, F.W.Fifield& D Kealey, 5th Ed. Blackwell Science, 2000.
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork,2003.
8. Instrumental Methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, 1986.
9. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
10. Quality in Totality – Parag Diwan, Deep & Deep Publications, 1st ed., 2000.

SEMESTER-III

LABORATORY-V

ACP-306 WET ANALYSIS LAB

Titrimetry

1. Determination of Ca^{2+} , Mg^{2+} , CO_3^{2-} & HCO_3^- 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 Dicloxacillin 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

ACP-307 ANALYTICAL INSTRUMENTATION 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.
2. GC study of two available drugs.

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

Recommended 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. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rdEdition Elbs Publication 1969.
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