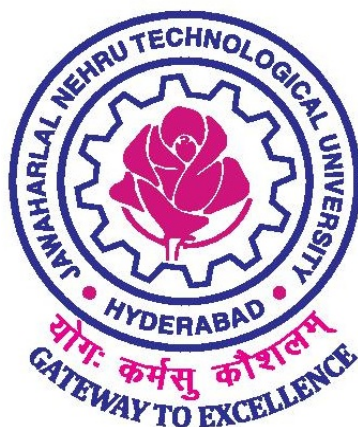


COURSE STRUCTURE AND SYLLABUS

M.Sc (Organic 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 ORGANIC 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	Organic Chemistry – III	25	75	4	-	4
2.	Core Course VII	Organic Chemistry – IV	25	75	4	-	4
3.	Core Course IX	Organic Chemistry - V	25	75	4	-	4
4.	Core Elective III	(i) Mechanism of Drug action (ii) Bio Inorganic Chemistry	25	75	4	-	4
5.	Open Elective III	(i) Drug Design and Synthesis (ii) IPR	25	75	4	-	4
6.	Laboratory V	Organic Chemistry Lab-II	25	50	-	6	3
7.	Laboratory VI	Pharmaceutical Technologies Lab	25	50	-	6	3
8.	Seminar	Seminar	--	50	-	3	2
	Total		175	525	20	15	28

IV Semester		Int. Marks	Ext. Marks	L	P	C
1.	Comprehensive Viva-Voce		100			4
2.	Project Work Review	50	-	-	8	2
3.	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

OCT-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. Sunderberg, 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

OCT-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:

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

OCT – 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: Michaeli's -Menten kinetics.

UNIT V: Solid State Chemistry

(12 Hrs)

Crystalline nature

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

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

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

OCT-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:

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. Pietrazyk 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

OCT-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 Hennan 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 etal.
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
15. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleman
16. Drug design By E.J. Arienes
17. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
18. Medicinal chemistry An introduction By Gareth Thomas

SEMESTER-I

OPEN ELECTIVE- I

OCT-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

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

OCT-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

OCP – 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

OCP – 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

OCT-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, Petero-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 hetero cyclic systems with more than one hetero atom. Synthesis, properties and applications of Pyrazole, Imidazole, Benzimidazoles, Purines, Oxazole, Thiazole, Isooxazole, 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

OCT-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

OCT-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

OCT – 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

AOCT-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, alkalis, 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

OCT-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

OCT-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

OCP-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

OCP-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

OCT-301: ORGANIC CHEMISTRY-III

Unit I: Oxidations & Reductions: (12 Hrs)

Oxidations :

Introduction, Different oxidative processes. Alcohols to Carbonyl compounds, Dimethyl Sulphoxide and its modifications (Swern oxidation), Manganese dioxide. Alkenes to Epoxides Peroxide induced epoxidation – epoxidation by H₂O₂, hydroperoxides and peroxyacids, Jacobson epoxidation, Shi epoxidation. Alkenes to Diols: Oxidation by Potassium Permanganate and Osmium tetroxide, Prevost oxidation and Woodward oxidation. Oxidative cleavage of 1,2-diols: Periodic acid, lead tetra acetate. Oxidation of allylic and benzylic C-H bonds. DDQ, SeO₂.

Reductions:

Introduction, Different reductive processes. Catalytic hydrogenation: Homogeneous (Wilkinson) and Heterogeneous Catalytic reductions (Noyori asymmetric hydrogenation). Dissolving metal reductions including Birch reduction. Non metallic reductions: Wolf Kishner reduction and Diimide reduction. Metal hydride reductions: Nucleophilic metal hydrides—LiAlH₄ and NaBH₄. Use of tri-n-butyltin hydride. Enzymatic reduction - Baker's yeast.

Unit II: Synthetic strategies (12 Hrs)

Introduction – Target selection, Retro synthesis – Disconnection approach with suitable examples (Simple molecules). Functional group interconversions (FGI) disconnection product. Chemo selectivity; Regio selectivity and Stereo selectivity with examples. Linear and consecutive synthesis.

Unit III: Modern Synthetic reactions (12 Hrs)

Heck reaction, Suzuki reaction, Sonogashira reaction, Shapiro reaction, Baylis-Hillman reaction, Umplong-use of dithio acetals, Ugi reaction, Wittig and Horner-Emmons olefination, Julia-Lythgoe olefination, Eishenmosher-Tenabe fragmentation and Shapiro reaction, Aza-Cope and Azawitting reaction. Buchwarld-Hertwig reaction. Stille coupling, Mc.murry coupling, Mukiyama aldol reaction, Mitsunobu reaction, Ritter reaction, Sakurai reaction. Ring closing meta thesis-Grubbs catalyst.

UNIT IV: Natural products-I (12 Hrs)

Alkaloids-source and classification, extraction and general methods for determining structure. Structure Determination of papaverine and Quinine. Steroids-source and classification of steroids and structure Elucidation of Cholesterol. Nomenclature of prostaglandins classification, Biosynthesis, metabolism and pharmacological action and synthesis of PGE₁, PGE₂ and PGF_{2 α} . Terpenoids: Structure synthesis and pharmacological importance of α -Terpinol, Camphor.

Unit V: Advanced Natural products (12 Hrs)

Stereo chemical structures, synthesis and pharmacological importance of the following

1. Alkaloids (Reserpine and Camptothecin, Morphine and Codeine and Thebaine)
2. Terpenoids (Abeitic acid, Taxol, Azadirachtin)
3. Steroids (Sex hormones) (Testosterone, Progesterone, Estrone), Adrosterone
4. Antibiotics(streptomycin, Tetracyclins)

Recommended Books:

1. Advanced organic chemistry, 4th edition (Wiley Inter Science, New York, 1993) by Jerry March
2. A guide book to mechanism in organic chemistry by Peter Sykes (FLBS).
3. Organic Synthesis-The disconnection approach by S Warren
4. Organic Synthesis by C Willis and M Willis
5. Problems on organic synthesis by Stuart Warren
6. Textbook of organic chemistry, Vol II by I L Finar
7. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
8. An introduction to the chemistry of terpenoids and steroids, by William templeton
9. Systematic identification of flavonoid compounds by Mabry & Markham
10. Biosynthesis by T.A.Geismann
11. Biosynthesis of organic compounds- Bernfield
12. Classics in total synthesis K C Nicolaou and E J Sorenson

SEMESTER-III

CORE COURSE VIII

OCT-302: ORGANIC CHEMISTRY-IV

UNIT – I: Principles of asymmetric synthesis (12 Hrs)

Introduction and terminology: Topicity in molecules homotopic, stereo heterotopic (Enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria.

Pro chirality nomenclature: pro-R, Pro-S, Re and Si.

Selectivity in synthesis: Stereospecific reactions (substrate stereo selectivity). Stereo selective reactions (Products stereo selectivity): Enantio selectivity and diastereo selectivity.

Conditions for stereo selectivity: Symmetry and transition state criteria. Kinetic and thermodynamics control. Methods for inducing enantio and diastereo selectivity.

Analytical methods: % Enantiomer excess and % enantio selectivity optical purity, % diastereomeric excess and % diastereo selectivity. Techniques for determination of enantio selectivity. Specific rotation, chiral ^1H NMR, chiral lanthanide shift reagents and chiral HPLC.

UNIT-II: Methodology of Asymmetric synthesis-I (12 Hrs)

Classification of Asymmetric reactions into Substrate controlled, Chiral Auxiliary controlled, Chiral reagent controlled and Chiral catalyst controlled.

Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α -alkylations of chiral enolates, azlones, imines and hydrazones, chiral sulfoxides. 1,4-asymmetric induction and Prelog's rule. Use of chiral Auxiliaries in Diels Alder and Cope reactions.

UNIT-III: Methodology of Asymmetric synthesis-II (12 Hrs)

1. Chiral reagent controlled asymmetric synthesis; asymmetric reactions using BINOL, asymmetric hydroboration using IPr_2BH and IPrBH_2 . Reductions with CBS reagent.

2. Chiral; catalyst controlled asymmetric synthesis; Sharpless, Jacobsen and Shi asymmetric epoxidations, Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Chiral catalyst controlled Diels-Alder and Michael reactions, enzyme mediated enantio selective synthesis;

3. Asymmetric aldol reaction; diastereo selective aldol reaction and its explanation by Zimmerman-Traxel model. Auxiliary controlled aldol reaction. Double diastereo selection-matched and mis-matched aldol reactions.

UNIT IV: ^{13}C NMR SPECTROSCOPY (12 Hrs)

CW and PFT techniques. Types of ^{13}C NMR spectra; uncoupled, proton-decoupled, single frequency off-resonance decoupled (SFORD) and selectivity decoupled spectra.

^{13}C chemical shift, factors affecting the chemical shifts, chemical shifts of organic compounds, calculation of chemical shift of alkanes, alkenes and alkynes.

Homo nuclear (^{13}C - ^{13}C) and hetero nuclear (^{13}C - ^1H and ^{13}C - ^2H) coupling. Applications of ^{13}C - NMR spectroscopy: Structure determination, stereo chemistry, reaction mechanisms and dynamic processes in organic molecules.

¹³C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

UNIT-V: 2D-NMR Techniques

(12 Hrs)

Principles of 2D-NMR, classification of 2D-Experiments. 2D-j resolved spectroscopy-Homo nuclear and hetero nuclear 2D-J resolved spectroscopy. Correlation spectroscopy (COSY) Homo COSY (HMQC), long range ¹H-¹³C COSY (HMBC); NOESY and 2D-INADEQUATE experiments and their applications.

Recommended Books:

1. Carbon -13 NMR of organic chemists by GC LEVY and O L Nelson
2. Modern NMR techniques for chemistry research by Andrew E Derome
3. Stero synthesis in organic synthesis by R S Ward.
4. Assymmetric Synthesis by Nogaradi.
5. Assymmetric organic reactions by JD Morrison and HS Moscher.
6. Spectroscopic identification of organic compounds by R.M. Silverstien, G.C. Bassler and
7. T.B. Morril

SEMESTER-III

CORE COURSE IX

OCT- 303: ORGANIC CHEMISTRY-V

UNIT-I:

a) Protecting groups: (12 Hrs)

a) Protection of alcohols by ether, silyl ether and ester formation b). Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, t-butyloxycarbonyl, triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation

b) New techniques and concepts in organic synthesis

1. **Techniques in peptide synthesis:** Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2) **Solid phase oligodeoxynucleotide synthesis:** Triester pathway and phosphoramidite pathway

3) **Oligosaccharide synthesis:** convergent and linear oligosaccharide synthesis

4) **Phase Transfer catalysis:** Onium and crown ethers as PTC.

5) **Tandem Synthesis:** Tandem reactions; conjugate additions, Aldol reaction, polymerization - cyclisation, electrocyclic- Diels Alder reaction.

6) **Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations

Unit II: Organo metallic reagents (12 Hrs)

Principle and preparation, Properties and applications of the following Metallo organic synthesis with mechanistic details of Grignard reagents; Organolithium reagents, Organo copper reagents, Organo boron reagents – Hydroboration.

UNIT-III: Green chemistry (12 Hrs)

Basic principles of Green synthesis. Green catalysts-Acid catalysts-Oxidation catalysts, basic catalysts, polymer supported catalysts. Darzens reaction, Williamsons synthesis Wittig reactions. Ionic liquids as green solvents-green solvents, reactions in acidic ionic liquids and basic ionic liquids (Hydrogenation, Diels Alder reaction, o-Alkylation and N-alkylation, Methylene insertion reactions.)

Microwave induced and ultra sound assisted Green synthesis

Microwave assisted reactions in water-Hoffmann elimination, hydrolysis, oxidation, saponification reactions. Microwave assisted reactions in organic solvents-esterification reactions, fries rearrangement, ortho ester Claisen rearrangement, diels alder reaction, decarboxylation. Microwave solvent free reactions (solid state reactions)-deacetylation deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

UNIT-IV:

(12 Hrs)

Biosynthesis of natural products

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of biosynthetic precursors, feeding experiments–use of radioisotopes. Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods.

Structure determination and stereochemistry of natural products by chemical methods

Determination of structure and stereochemistry of Flavones, Isoflavones and Coumarin.

UNIT-V:

(12 Hrs)

Concepts & applications involved in catalysis:

Introduction to catalysis, homogenous & Heterogeneous catalytic reactions. Physisorption, chemisorption. Adsorption Isotherms. Derivation of Langmuir adsorption isotherm (single component).

Methods of preparation of catalysts:

Classification of catalysts and support materials. Impregnation, precipitation, solid-solid mixing. Filtration. Drying, pelletization, calcination. Equipment for these processes.

Major Reactions: Oxidation / reduction, isomerization, cracking, hydrogenation, water gas shift reaction, Ammonia synthesis, Fisher - Tropsch synthesis, Hydroformylation, Carbonylation, Polymerization, Cracking, hydrotreatment, Alkylation, Reforming, phase transfer catalysts.

Recommended Books:

1. Catalysis by Kuriacose
2. Basic Principles in applied catalysis by Manfredlaerns
3. Organic synthesis in water. By Paul A. Grieco Blackie.
4. New trends in Green chemistry By V.K. Ahluwalia and Renu Aggarwal.
5. Some modern methods of organic synthesis by W. Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
8. Organic synthesis by Robert E Ireland
9. Total synthesis of natural products: the Chiron approach by S. Hanessian
10. Biosynthesis by T.A. Geismann
11. Biosynthesis of organic compounds- Bernfield

SEMESTER-III

CORE ELECTIVE-III

OCT-304.1: MECHANISM OF DRUG ACTION

UNIT-I: Basic concepts of mechanism of drug action (12 Hrs)

Different types of classification of drugs, introduction to macro molecular targets-structure of bacterial cell wall and folate metabolism in bacteria. Structure of Human cell-importance of membrane lipids, proteins and carbohydrates. Nucleic acids as targets. Introduction to immune system and structure of neurons, definition and examples of agonists, antagonists neurotransmitters, receptors and classification of receptors. Introduction to ion channels and their functions, Solubility, permeability, drug efficiency, selectivity, Toxicity, ADMEJ properties, drug likeliness, Lipinski's rules.

UNIT-II: Drugs acting on metabolic processes and cell walls (12 Hrs)

Drugs acting on metabolic processes:

Antifolates-Discovery and mechanism of action of sulfonamides, sulfones and diamino pyrimidines. Synthesis of sulphamethoxazole, sulfaguanidine, dapsone and trimethoprim.

Drugs acting on cell walls

β -lactams-mechanism of action of penicillins and cephalosporins cephalosporin-c, cefalaxin and cycloserine. β -lactamase inhibitors-structural formulae of sulbactam and clavulanic acid and their mode of action. Structure of polymyxins and their action on cell membranes. Synthesis of penicillin-G.

UNIT-III: Drugs acting on ion channels and other receptors (12 Hrs)

Drugs acting on Ca^{+2} , Na^{+} and K^{+} channels and their mode of action. Synthesis of Nifedipine, Diltiazem, Tetracaine and Amethocaine.

Drugs acting on receptors:

α -adrenergic-receptor agonists and antagonists-Biosynthesis of catecholamine. Structural formulae of APC, Benexetramine and synthesis of epinephrine, nor-epinephrine, methyl dopa and terazosin. Biological activity of these drugs.

β -adrenergic receptor agonists and antagonists-Synthesis and pharmacological activity of salbutamol, terbutalin, propranolol, metoprolol and atenolol.

Cholinergic receptor agonists and antagonists- Biosynthesis of acetylcholine, synthesis of acetylcholine and succinylcholine. Structural formulae of Atropine, Nicotine and Tubocurarine. Biological activity of these drugs.

Dopamine receptor agonists and antagonists-Biosynthesis of Dopamine. Synthesis and pharmacological activity of L-Dopa and Chlorpromazine.

Histamine receptor agonists and antagonists-Synthesis and pharmacological action of Histamine, chlorpheniramine, Ranitidine and Cimetidine. Structural formula of Promethazine and its importance.

UNIT-IV: Drugs acting on genetic materials and other receptors (12 Hrs)

a) Drugs acting on genetic material:

i) **DNA-inter chelating agents-anticancer and antimalarial agents:** Structural formulae of daunomycin, adriamycin and ellipticine. Synthesis of amsacrine, nitracrine, quinacrine and chloroquine.

ii) **DNA-binding and nicking material;**

- Antiprotozoal drugs-synthesis of metronidazole, and dimetrizole.
- iii) **DNA-Topoisomerase inhibitors;**
Antibacterial agents-synthesis of ciprofloxacin and norfloxacin.structural formulae of ofloxacin and lomefloxacin.
 - iv) **DNA –Polymerase inhibitors:**
Antiviral agents-synthesis of AZT and acyclovir.introduction to interferons.
 - v) **Inhibitors of transcribing enzymes:** Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.
 - vi) **Drugs interfering with translations.** Antibacterial drugs-structural formulae of erythromycin, chloromycitin, tetracyclines and amino glycosides. Synthesis of chloromycetin.

UNIT-V: Drugs acting on Specific enzymes and immune system (12 Hrs)

- A) **Drugs acting on specific enzymes:**
Inhibitors of glucosidase, ACE, H⁺, K⁺, ATPase and carbonic anhydrase enzymes.
Synthesis and medicinal importance of captopril, enalapril and omeprazole.
- B) Inhibition of prostaglandin synthase: Synthesis and medicinal use of oxyphenbutazone, Ibuprofen, Diclofenac, etodolac, piroxicam.
- C) **Drugs acting on immune system:**
 - i) Immuno suppressing agent-structural formula and mechanism of action of cyclosporin.
 - ii) Imuno enhancers-use of vaccines and structural formula of Levamisol.

Recommended Books:

- 1.Burger's medicinal chemistry and Drug discovery.By Manfred B.Wolf.
- 2.Introduction to medicinal chemistry .By Graham Patric.
- 3.Introduction to drug design.By R.B.silverman
- 4.comprehensive medicinal chemistry.vol 1-5 By Hanzsch.
- 5.principles of medicinal chemistry.By William foye .
- 6.Biochemical approach to medicinal chemistry.Bythomas Nogrady.
7. Pharmaceutical chemistry and drug synthesis By Roth and Keelman.
- 8.Drug design ByE.J. Arienes.
- 9.principles of medicinal chemistry. vol1&11 BY.Kadam etal .
- 10.Medicinal chemistry an introduction.By Gareth Thomas.

SEMESTER-III

CORE ELECTIVE-III

OCT-304.2: BIOORGANIC CHEMISTRY

UNIT-I: Enzymes and their action (12 Hrs)

Introduction to enzymes. Transition state theory. Acid-Base catalysis. Covalent catalysis— Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. Examples of some typical enzyme mechanisms for (1) Triose phosphate isomerase, (ii) α -chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease.

UNIT-II: Enzyme Models and Enzymatic transformations (12 Hrs)

Introduction — Biomimetic chemical approach to biological systems-Enzyme models Advantage of enzyme models. Requirements necessary for the design of enzyme models. Host-Guest complexation chemistry. Examples of some host molecules-Crown ether cryptanes, cyclodextrins. Cyclodextrin based enzyme models-Valixarenes, ionophores, micelles and synzymes (synthetic enzymes) — chiral recognition and catalysis. Introduction to industrial enzymes. Enzymatic synthesis of α -amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of carboxylic acids, esters and alcohols - Transesterification. Amine resolution-use of oxido-reductase. C-C bond formation using enzymes-asymmetric cyanohydrin formation and asymmetric aldol condensations.

UNIT-III: Recombinant DNA (12 Hrs)

Introduction to genetic engineering. Recombinant DNA technology-restriction endonuclease, cloning, linkers, adaptors. Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples. Principles of finger printing technology- Site directed mutagenesis.

UNIT-III: Fermentation technology (12 Hrs)

Fermentation technology: Introduction to fermentation. Industrial fermentation. Advantages and limitations of fermentation. Production of drugs and drug intermediates from fermentation examples. Chiral hydroxy acids, vitamins, amino acids, β -lactam antibiotics. Precursor fermentation and microbial oxidation and reductions.

UNIT-V: Coenzymes (12 Hrs)

Introduction. Co factors — cosubstrates — prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH) ii) Flavin adenine nucleotide FAD, FADH₂ and iii) Flavin mononucleotide (FMN, FMNH₂) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Recommended Books

1. Concepts in biotechnology by D. Balasubramanian & others
2. Principles of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Chirotechnology by R.Sheldon

SEMESTER-III

OPEN ELECTIVE-III

OCT- 305.1 DRUG DESIGN AND SYNTHESIS

UNIT- I: Drug Design - A Rational Approach (12 Hrs)

1. Introduction: Principles of drug discovery, factors governing drug design, rational approach to drug design, Drug design - the method of variation, drug design through disjunction and conjunction.

2. Physico-chemical factors: Introduction, structurally - specific and non-specific drugs, factors governing ability of drugs to reach active site, distribution, excretion. 3. Isosterism and Bio-isosterism.

UNIT-II: molecular modeling (12 Hrs)

A. Structure and analog based approaches virtual screening, pharmacophore, docking and de novo drug design

B. Lead modification strategies: Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion or contraction, ring variation and variation and position on hetero atoms, ring fusion, simplification of the lead, rigidification of the lead. Discovery of oxamiquine, salbutamol, cimitidine and captopril structure activity relationship studies in sulfa drugs, benzodiazapines and taxol analogs. Principles of molecular modeling.

UNIT III: Quantitative structure -activity relationship studies (12 Hrs)

Introduction to Quantitative-structure-activity relationship studies. QSAR parameters- P_{ka} , Hammett constants, π (lipophilicity) constants and Taft's constants. Linear or non-linear relationship between Hammett substituent constant biological activity. Linear or non linear relationship between $\log p$ (lipophilicity constant) and biological activity. Lipinski's rule of five multiparameter QSAR-Hansch analysis, Craig's plot, Topliss method and cluster analysis, case studies to be disclosed.

UNIT-IV: General Pathways of Drug Metabolism: (12 Hrs)

Meaning of metabolism, factors affecting metabolism: i) genetic factors
ii) Physiological factors
iii) Pharmaceutical factors
iv) Drug interactions.

Phases of metabolism or metabolic pathways with some examples of the following:

- Hydroxylation: eg. Acetanilide, Nitrazepam, Meprobamate.
- Reduction: eg. Prontosil, Chloralhydrate.
- Hydrolysis: eg. Cocaine, Procaine.
- Oxidation/Reduction: eg. Prostaglandins
- Conjugations: eg. Glucuronide formation, sulfate formation, acetylation, methylation and conjugation with amino acids.
- O-Dealkylation and N-Dealkylation: eg. Codeine, Mephobarbital and Chlorpromazine.

UNIT-V: Chiral Drugs and IPR (12 Hrs)

A) Chiral synthesis and Activity of the following Drugs:

S-Ibuprofen, S-Naproxen, Levocetazine, 2S-Verapamil, S,S-Ethambutol, R-Indacrinone,

B) Intellectual Property Rights

Definition, scope and different forms of IPR. Patents, definition, types, contents of patent, claims and types of claims, requirements for patenting, restrictions and the power of patents.

Recommended books:

- 1 Wilson Gisvold, Textbook of Organic Medicinal and Pharmaceutical Chemistry
- 2 Ashutoshkar, Medicinal Chemistry
- 3 Ed. Burger, Medicinal Chemistry, Volume 1, 2 & 4.
- 4 Introduction to Medicinal chemistry, by Graham Patrick.
- 5 Drug design by E.J.Ariens.
- 6 Strategies of organic drug design synthesis and design by Daniel Ledneiser.
- 7 Principles of Medicinal Chemistry Vol I & II by Kadam et al
- 8 Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
- 9 Principles of Medicinal Chemistry Vol I & II by Kadam et al
- 10 Medicinal chemistry An introduction by Garreth Thomas
- 11 Organic and Pharmaceutical chemistry By Delgrado
- 12 Organic Pharmaceutical chemistry By Harikishan singh
- 13 How to Practice GLP, PP Sharma , vandana Publications ,2000,New Delhi.
- 14 Applying ISO-9000 Quality Management systems, International Trade Centre publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust

SEMESTER-III

OPEN ELECTIVE-III

OCT- 305.2 Intellectual Property Rights and Quality Management

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: Choosing the methods – standard methods, official methods, literature methods. Validation of new methods – Comparison of analytical methods, ruggedness testing of methods, writing analytical methods, modification of analytical methods.– ICH guidelines for method validation, Comparison of analytical methods, 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 labelling, 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. Patents, definition, types, contents of patent, claims and types of claims, requirements for patenting, restrictions and the power of patents.

Recommended books:

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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,Intrnational Trade Centre publishing,UNCTAD/WTO.Geneva,Switzerland,Indian Edition Printed by D.L.Shah Trust

SEMESTER-III

LABORATORY-V

OCP – 306 ORGANIC CHEMISTRY LAB-II

1. Separation and identification of binary mixtures of organic compounds.
2. Synthesis of organic compounds(Multistep synthesis)
 - a) Benzillic acid
 - b) Benzanilide from Benzophenone
 - c) Caprolactam
 - d) vanilyl alcohol from vaniline
 - e) 2 and 4-Nitrophenol distillation(Nitration and separation by steam distillation)
 - f) O-chloro Benzoic acid from phthalic anhydride.

LABORATORY-VI

OCP-307 ORGANIC CHEMISTRY LAB-III

1. Isolation and purification of the following natural products
 - a) Piperidine from black pepper
 - b) Caffeine from Tea leaves
 - c) Eucalyptous oil.
 - d) Lycopene from tomatoes
2. Determination of TLC and RF value of organic compounds
3. Identification and interpretation of unknown organic compounds by spectra, viz., UV, IR, NMR & mass spectral analysis.
4. Synthesis of important drugs