COURSE STRUCTURE AND SYLLABUS

M.Sc (ORGANIC CHEMISTRY)

CHOICE BASED CREDIT SYSTEM (CBCS)

(With effect from 2022-23)

CENTRE FOR CHEMICAL SCIENCES AND TECHNOLOGY

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

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY HYDERABAD

KUKATPALLY, HYDERABAD-500085, TELANGANA

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

I YEAR

Subject Code	I semester	Course Title	Int. Marks	Ext. marks	L	P	C
1OCPC101	Program Core I	Organic Chemistry – I	40	60	3	-	3
1OCPC102	Program Core II	Inorganic Chemistry	40	60	3	-	3
1OCPC103	Program Core III	Physical Chemistry-I	40	60	3	-	3
1OCPE104	Program Elective I	(i) Principles of Analytical Chemistry (ii) Bio Molecules	40	60	3	-	3
1OCOE105	Open Elective I	(i) Applied Chemistry (ii) Computers and mathematics	40	60	3	-	3
1OCL106	Laboratory I	Inorganic Chemistry Lab	40	60	-	6	3
1OCL107	Laboratory II	Physical Chemistry Lab-I	40	60	-	6	3
1OCS108		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

Subject Code	II semester	Course Title	Int. Marks	Ext. Marks	L	P	C
2OCPC209	Program Core IV	Concepts in Organic Chemistry	40	60	3	-	3
2OCPC210	Program Core V	Instrumental Methods of Analysis	40	60	3	-	3
2OCPC211	Program Core VI	Physical Chemistry-II	40	60	3	-	3
2OCPE212	Program Elective II	(i) Spectroscopic Methods of Analysis- I (ii) Applied Analysis	40	60	3	-	3
2OCOE213	Open Elective II	(i) principles of chemical engineering (ii) Physical Organic Chemistry	40	60	3	-	3
2OCL214	Laboratory III	Organic Chemistry Lab –I	40	60	-	6	3
2OCL215	Laboratory IV	Physical Chemistry Lab-II	40	60	-	6	3
2OCS216		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

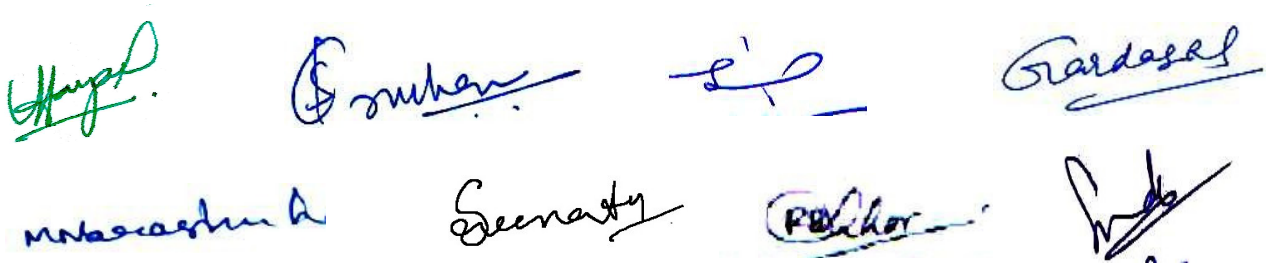
II YEAR

Subject Code	III semester	Course Title	Int. Marks	Ext. Marks	L	P	C
3OCPC317	Program Core VII	Organic Chemistry – III	40	60	3	-	3
3OCPC318	Program Core VIII	Organic Chemistry – IV	40	60	3	-	3
3OCPC319	Program Core IX	Organic Chemistry - V	40	60	3	-	3
3OCPE320	Program Elective III	(i) Mechanism of Drug action (ii) Bio Inorganic Chemistry	40	60	3	-	3
3OCOE321	Open Elective III	(i) Drug Design and Synthesis (ii) IPR & Quality Management	40	60	3	-	3
3OCL322	Laboratory V	Organic Chemistry Lab-II	40	60	-	6	3
3OCL323	Laboratory VI	Synthesis of Organic compounds and Chromatography	40	60	-	6	3
3OCS324		SEMINAR		50	3	-	2
	Total		**280**	**470**	**18**	**12**	**23**

Subject Code	IV Semester	Int. Marks	Ext. Marks	L	P	C
	Dissertation work review I	**0**	0	0	0	0
4OC425	Dissertation work review II	50	-	-	4	2
4OC426	Dissertation Evaluation (Viva Voce)	-	100	-	18	9
	Total	**50**	**100**		**22**	**11**

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

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



SEMESTER-I

PROGRAM CORE –I

1OCPC01: ORGANIC CHEMISTRY – I

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

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

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

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

UNIT II: Stereochemistry-I **(12 Hrs)**

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

UNIT – III: Heterocyclic Compounds I **(12 Hrs)**

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

UNIT –IV **(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 A_1, B_1, B_2, B_6, C, Biotin and E.

UNIT – V Reaction Intermediates and Rearrangements: (12 Hrs)

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

b) Molecular rearrangements

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

Recommended books:

1. Stereochemistry of Organic Compounds by Ernest L. Eliel, Samuel H. Wilen.
2. Stereochemistry of organic compounds: Principles and Applications by D. Nasipuri.
3. Heterocyclic Chemistry by T.L. Gilchrist.
4. Organic Chemistry by Clayden.
5. Organic Reaction Mechanisms by V.K. Ahluwalia & Rakesh K. Parashar.

Further reading:

1. Benzofurans by A. Mustafa.
2. Heterocyclic Chemistry by J.A.Joule, K.Mills and G.F.Smith.
3. The Chemistry of Indole by R. J. Sunderberg.
4. An introduction to the chemistry of heterocyclic compounds by R.M.Acheson.
5. Advanced Organic Chemistry: Reactions, Mechanisms and Structure by Jerry March
6. Reaction Mechanism In Organic Chemistry By Mukherjee And Singh
7. Guide Book to mechanism in Organic Chemistry by Peter Sykes.
8. Organic Chemistry by Graham Solomous and Craig B Fryhle
9. Organic Chemistry by RT Morrison and RN Boyd.
10. Organic Chemistry, Vol. 2 by I.L. Finar.
11. Organic Chemistry: Structure and Reactivity by Ege, Seyhan N.

SEMESTER-I

PROGRAM CORE –II

1OCPC02: INORGANIC CHEMISTRY

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

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

Metal Ions in Biological Systems:

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

UNT – II: Coordination Equilibria (12 Hrs)

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

UNIT – III: Reaction Mechanism: (12 Hrs)

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

Nucleophilic Substitution reactions of Octahedral Complexes:

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

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

Nucleophilic Substitution Reactions of Square planar Complexes*:*

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

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

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

UNIT – V: Metal Clusters (12 Hrs)
Carbonyl Clusters
a) Ligational properties of CO: Donor (HOMO) and Acceptor (LUMO) Molecular Orbitals of CO Bonding modes of CO: Terminal and Bridging-Bonding - Classification into mononuclear, Binuclear, Trinuclear and Tetranuclear carbonyls. Structures of Ni $(CO)_4$, Cr $(CO)_9$, $Mn_2(CO)_{10}$, $Fe_2(CO)_9$ and $Co_2(CO)_8$-Eighteen Electron Rule in Metal Carbonyls.
b) 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.

Further reading:

1. BioInorganic Chemistry- K.Hussain Reddy
2. Selected Topics in Inorganic chemistry madan,Malik,Tuli S.Chand publications.
3. Inorganic reaction Mechanism- F.Basolo & R.G.Pearson, New York.
4. Inorganic Chemistry- Keith F.Purcell & John C.Kotz Holt- Saunde International Edition.
5. Ligational aspects of diatomic molecules-Organometallic Chemistry R.C.Mehotra.

SEMESTER-I

PROGRAM CORE –III

1OCPC03: PHYSICAL CHEMISTRY – I

UNIT- I: Thermodynamics-1 (12 Hrs)

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

Third law of thermodynamics:

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

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

Unit-II: Electrochemistry (12 Hrs)

Ionics:

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

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

Electrodics:

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

Unit-III: Quantum chemistry (12 Hrs)

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

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

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

UNIT IV: Chemical Kinetics **(12 Hrs)**

Theories of reaction rates

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

Complex Reactions

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

Homogeneous catalysis

Introduction to homogeneous and heterogeneous catalysis with examples in homogeneous catalysis.
Introduction to enzyme catalysis: Michaeli's -Menten kinetics.

UNIT V: Solid State Chemistry **(12 Hrs)**

Crystalline nature

Classification. Crystal defects. Perfect and imperfect crystals. Classification of imperfections. Point defects. Schottky defects. Frenkel defects. Line defects and plane defects. Electron diffraction, Bragg's law and applications, Band theory, band structure of metals, insulators and semiconductors.
Superconductivity. Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect. Types of superconductors. Theories of super conductivity-BCS theory, high temperature superconductors.

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

Further reading:

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

SEMESTER-I

PROGRAM ELECTIVE- I

1OCPE04.1: 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.

Suggested books:

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

Further reading:

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

SEMESTER-I

PROGRAM ELECTIVE- I

1OCPE04.2: BIOMOLECULES

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

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

UNIT-II. Nucleic acids: (12 Hrs)

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

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

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

UNIT-IV: Vitamins: (12 Hrs)

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

UNIT-V: Introduction to Drugs (12 Hrs)

Introduction, Classification, examples of natural and synthetic drugs.

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

Suggested books:

1. Enzyme structure and mechanism by Fersht and Freeman

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

Further reading:

1. Biotransformations in Organic Chemistry by K Faber.
2. Principles of biochemistry by Horton & others.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.

SEMESTER-I

OPEN ELECTIVE- I

1OCOE05.1: 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

CrystalizationTechniques: Different kinds of crystallization, Single crystal generation

b) Industrial safety:

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

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

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

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

UNIT IV: Fuel Technology **(12 Hrs)**

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

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

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

Types of polymerization –anionic, cationic, free radical, coordinate polymerization ring opening.

Types of initiators-Free radical, Anionic, 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.

Suggested Books:

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

Further reading:

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

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SEMESTER-I

OPEN ELECTIVE- I

1OCOE05.2: COMPUTERS AND MATHEMATICS

UNIT-I: Computer basics: (12 Hrs)

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

UNIT-II: Arithmetic operators: (12 Hrs)

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

UNIT-III: Classifications: (12 Hrs)

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

Unit-IV: Differential Calculus: (12 Hrs)

Functions-continuity and differentiability, Rules for differentiation. Sums, products and quotients of functions. The chain rules. Differentiation of algebraic, exponential logarithmic and composite functions. First order differential equations- separable variables. Homogenous and linear differential equations. Linear second order differential equations-solutions for homogenous equations. Higher order derivatives. Maxima and minima. Partial differentiation and meaning of total derivative exact and inexact differentials **Integral Calculus:** Basic rules for integration. Methods for evaluating integrals-the substitution method, use of partial fractions, integration by parts. Definite integrals.

UNIT V: Introduction to statistics (12 Hrs)

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

Suggested Books:

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

SEMESTER-I

LABORATORY-I

1OCL06: INORGANIC CHEMISTRY LAB

Quantitative Analysis: Preparation of the following inorganic complexes.

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

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

Suggested Books

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

SEMESTER-I

LABORATORY-II

1OCL07: PHYSICAL CHEMISTRY-LAB-I

Acid Base Titrations

Conductometry

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

Potentiometry

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

Chemical Kinetics

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

Suggested Books:

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

SEMESTER-II

PROGRAM CORE IV

2OCPC08: 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 diasteromers & enantiomers, factors affecting conformational stability and conformational equilibrium-attractive and repulsive interactions.

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– π^*, π – π^* transitions, Norrish type I and Norrish type II cleavages, Peterno-Buchi reactions, rearrangements of α,β,-unsaturated ketones and cyclic hexadienes, photochemistry of P-Benzoquinones, photochemistry of unsaturated system – olefins, cis-trans isomerism and addition acetylenes dimerisation, dienes – photochemistry of 1,3- butadienes (2+2) additions leading to cage structures and photochemistry of cyclohexadienes, Di-π methane rearrangement

Unit 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, Benzimidazole, Purine, Pyrimidine, Oxazole, Isooxazole, Oxadiazole, Thiazole, Thiadiazole, Triazole, Tetrazole, Pyradazine, Pyrazine, Triazine.

Suggested Books:

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

Further reading:

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

PROGRAM CORE V

2OCPC09: ELECTRO ANALYTICAL TECHNIQUES.

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

Principle, Fundamental equations, measurement of conductance, Conductometric titrations.
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.
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: Polarographic Techniques (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: **Chromatographic Techniques-III** (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.

Suggested books:

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

SEMESTER-II

PROGRAM CORE VI

2OCPC10: 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 adsorption isotherms-study of kinetics of surface reactions catalysis by metals, semiconductor oxides-mechanism of heterogeneous catalytic reactions-the adsorption coefficient and its significance.

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

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

UNIT V: Quantum Chemistry-II (12 Hrs)

Particle in a box-one dimensional and three dimensional. Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles.
Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.
Cartesian, Polar and spherical polar coordinates and their interrelations
Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation.
Polar plots, contour plots and boundary diagrams.
Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations.

Suggested Books:

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

Further Reading:

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

SEMESTER-II

PROGRAM ELECTIVEII

2OCPE11.1: 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. Chromopores, auxochromes, Applications of UV spectroscopy to simple organic molecules like conjugated dienes, trienes, unsaturated carbonyl compounds and aromatic compounds. woodward-Fieser rules.

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

Range & Nomenclature of IR, Theory of IR spectroscopy, modes of vibration, different types of vibration, Characteristic group frequencies: Alkanes, Alkenes, alkynes, cyclo alkanes and alkyl groups Aromatic compounds, alcohols, phenols ethers, cyclic ethers, amines, compounds containing carbonyl group, carboxylic acids, esters and lactones, anhydrides, nitro, nitroso and nitriles. Factors influencing vibrational frequencies, Instrumentation of IR Spectrophotometer
Raman Spectroscopy- Classical and Quantum theory of Raman effect, Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

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

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

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

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

Principles of Magnetic resonance, Resonance condition, Magnetic Moment & spin angular momentum, Larmor frequency, Proton Magnetic Resonance, Shielding Constants, chemical shifts, factors influencing chemical shifts, solvent shifts, Shielding & Deshielding phenomena, spin-spin coupling, coupling constants.
AX, AX_2, AX_3, AMX & AB Types of spectra, Methods of simplifying complex spectra. Double resonance technique, deuterium exchange, shift reagent, applications of PMR in structural determination-alcohols, amines, hydrogen bonding, keto-enol tautomerism, ^{19}F and ^{31}P NMR.

UNIT-V: Mass Spectrometry (12 Hrs)

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

Suggested books:

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

Further Reading:

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

SEMESTER-II

PROGRAM ELECTIVEII

2OCPE11.2: BIOPOLYMER CHEMISTRY

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

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

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

UNIT II: Biological membranes (12 hrs)

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

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

Binding of ligands and metal ions to macromolecules – one and n-euqivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H+ and CO2 . Bohr effect.

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

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA.

Types of RNA. Secondary structure of t-RNA Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method.

Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA.

DNA hybridization and hybridization probes. Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

UNIT V: Bioinformatics (12 hrs)

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

Suggested Books:

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

SEMESTER-II

OPEN ELECTIVE II

2OCOE12.1: PRINCIPLES OF CHEMICAL ENGINEERING

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

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

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

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

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

UNIT-III: Heat Transfer (12 Hrs)

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

UNIT-IV: Mass Transfer (12 Hrs)

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

UNIT-V: Chemical Reaction Engineering (12 Hrs)

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

Suggested Books:-

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

SEMESTER-II

OPEN ELECTIVE II

2OCOE12.2: PHYSICAL- ORGANIC CHEMISTRY

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

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiempirical methods and ab into and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels. Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions.

Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy.

Arrhenius equation, transition state theory. Uses of activation parameters, Hammonds postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and Selectivity principles

UNIT-II: Kinetic, isotopic, structural effects (12 Hrs)

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

UNIT-III: solvent, steric and conformational effects (12 Hrs)

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

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

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugality. The α-effect. - Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronsted catalysis. . nucleophilic and electrophilic

catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity: Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects, kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nucleophilicity and SN2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity.
Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and peri selectivity in pericyclic reactions.

UNIT-V: Supramolecular chemistry (12 Hrs)

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

Suggested books:

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

SEMESTER-II

LABORATORY III

2OCL13: ORGANIC CHEMISTRY LAB-I

Qualitative organic analysis

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

Synthesis of Organic molecules

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

Suggested books:

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

SEMESTER-II

LABORATORY IV

2OCL14: PHYSICAL CHEMISTRY LAB-II

Spectrophotometry

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

Polarimetry:

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

Adsorption and others:

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

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Suggested Books:

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

SEMESTER-III

PROGRAM CORE VII

3OCPC16: 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 H_2O_2, 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, SeO_2.

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: Nucleiphillic metal hydrides–$LiAlH_4$ and $NaBH_4$. 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, Sonagashira 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, Mitsnobu reaction, Ritter reaction, Sakurai reaction. Ring closing meta thesis-Grubbs catalyst. C-H Activation: Introduction, Rh catalyzed C-H Activation. Modern Organocatalysis (NHC, SUMO catalysis)

UNIT IV: Natural products (12 Hrs)

Alkaliods-source and classification, extraction and general methods for determining structure. Structure Determination of papaverine and Quinine. Sterooids-source and classification of steroids and structure Elucidation of Cholesterol. Nomenclature of prostaglandins classification, Biosynthesis, metabolism and pharmacological action and synthesis of PGE_1, PGE_2 and $PGF_{2\alpha}$.

Terpeniods: 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)

Suggested Books:

1. Advanced Organic Chemistry: Reactions, Mechanisms and Structure by Jerry March.
2. Modern Methods of Organic Synthesis by Carruthers.
3. A guide book to mechanism in organic chemistry by Peter Sykes.
4. Organic Synthesis-The disconnection approach by S Warren.
5. Organic Synthesis by C. Willis and M. Willis.
6. Organic Chemistry by Clayden.

Further reading:

7. Workbook for Organic Synthesis: The Disconnection Approach by Stuart Warren, Paul Wyatt.
8. Textbook of organic chemistry, Vol II by I. L. Finar.
9. Studies in Natural Products Chemistry: Structure and Chemistryby Atta-Ur-Rahman.
10. An introduction to the chemistry of terpenoids and steroids, by William Templeton.
11. Systematic identification of Flavonoids by Mabry & Markham.
12. Classics in total synthesis by K C Nicolaou and E J Sorenson.

SEMESTER-III

PROGRAM CORE VIII

3OCPC17: ORGANIC CHEMISTRY-IV

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

Introduction and terminology: Topicity in molecules homotopic, stereo hetereotopic (Enantiotopic and diastreotopic) 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). Strero selective reactions (Products stereo selectivity): Enatio selectivity and diastereo selectivity.

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

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

UNIT-II: Methodolgy of Assymetric synthesis-I (12 Hrs)

Classification of Assymetric 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 feikin-anh model.

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

UNIT-III: Methodolgy of Assymetric synthesis-II (12 Hrs)

1. Chiral reagent controlled asymmetric synthesis; asymmetirc reactions using BINALH, assymmetirc hydroboration using IPC_2BH and $IPCBH_2$. Reductions with CBS reagent.
2. Chiral; catalyst controlled asymmetric synthesis; sharpless, jacodsen and shi asymmetric epoxidations, sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and noypri catalysts. Chiral catalyst controlled diels-alder and Michael reactions, enzyme mediated enantio seletive synthesis;
3. Asymmetric aldol reaction; diostereo selective aldol reaction and its explanation byzimmerman-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; undecoupled, 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}CJ) and hetero nuclear (^{13}C-^{1}HJ and ^{13}C-^{2}HJ) coupling. Applications of ^{13}C-NMR spectroscopy: Structure detetermination, stereo chemistry, reaction mechanisms and dynamic processes in organic molecules.

^{13}C-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 ^{1}H-^{13}C COSY (HMBC); NOESY and 2D-INADEQUATE experiments and their applications. Structural elucidation of natural products using 2D NMR-. Coumarin-(7 Hydroxy-4 Methyl- coumarine), Camphor and Menthol.

Suggested Books:

1. Organic Spectroscopy by W.Kemp.
2. Spectroscopy of Organic Compounds by P.S.Kalsi.
3. Modern NMR techniques for chemistry research by Andrew E Derome
4. Selectivity in Organic Synthesisby R. S. Ward.
5. Assymetric Synthesis by Nogradi.

Further reading:

6. Assymetric organic reactions by J. D. Morrison and H. S. Moscher.
7. Spectroscopic identification of organic compounds by R.M.Silverstien,G.C.Bassler and T.B.Morril.

SEMESTER-III

PROGRAM CORE IX

3OCPC18: ORGANIC CHEMISTRY-V

UNIT-I: 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

Unit II: New techniques and concepts in organic synthesis (12 Hrs)

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 crwon ethers as PTC.
5) **Tandem Synthesis:**Tandem reactions; conjugateadditions,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 III: 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-IV: 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 liquida and basic ionic liquids (Hydrogenation, Diels Alder reaction, o-Alkylation and N-alkylation, Methylene insertion reactions.)

Microwave induced and ultra sound assited 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, decorboxylation. Microwave solvent free reacrtions (solid state reactions)-deacetylation deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

UNIT-V: 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, Cabonylation, Polymerization, Cracking, hydrotreatment, Alkylation, Reforming, phase transfer catalysts.

Suggested 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

Further reading:

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
8. Organic synthesis by Robert E Ireland
9. Total synthesis of natural products: the Chiron approach by S. Hanesian
10. Biosynthesis by T.A.Geismann
11. Biosynthesis of organic compounds-Bernfield

SEMESTER-III

PROGRAM ELECTIVE-III

3OCPE19.1: 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 chanels and their functions, Solubility, permeability, drug efficiancy, selectivity, Toxicity, ADMEJ properties, drug likelyness, 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 sulpha methaxazole, sulfagunadine, dapsone and trimethoprim.

Drugs acting on cell walls

β-lactams-mechanism of action of pencillins and cephalosporins cephalosporin-c, cefalaxin and cycloserine. β-lactamase inhibitors-structural formulae of sublactam and clavulanic acid and their mode of action. Structure of polymixins and their action on cell membranes. Synthesis of pencillin-G.

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

Drugs acting ion Ca^{+2}, Na^{+} and K^{+} channels and their mode of action. Synthesis of Nefedipine, 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, porpronolol, metaprolol and atenolol.

Cholinergic receptor agonists and antagonists- Biosynthesis of acetylcholine, synthesis of acetylcholine and succinylcholine. Styruuctural 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 Chloropromazine.

Histamine receptor agonists and antagonists-Synthesis and pharmacological action of Histamine, chlorophen eramine, Raniditine and Cimetidine. Structural formula of Impromidine 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 chioroquine.

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

Antiprotozoal drugs-synthesis of metronidazole, and dimetrizole.

iii) **DNA-Topoisomerase inhibitors**;
Antibacterial agents-synthesis of ciprofloxacin and norfloxcin.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, chioromycitin, 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 captropril, enalapril and omeprazole.

B) **Inhibition of prostaglandin synthase**:
Synthesis and medicinal use of oxyphenabutazone, Ibuprofen, Diclofenac, etodolac, piroxicam.

C) Drugs acting on immune system:

i) Immuno supressing agent-structural formula and mechanism of action of cyclosporin.

ii) Imuno enhancers-use of vaccines and structural formula of Levamisol.

Suggested Books:

1. Burger's medicinal chemistry and Drug discovery by Manfred B.Wolf.
2. An introduction to medicinal chemistry by Graham Patric.
3. The Organic Chemistry of Drug Design and Drug Action by R.B.silverman
4. Comprehensive medicinal chemistry by Hanzsch.

Further reading:

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 By E.J. Arienes.
9. Principles of medicinal chemistry. By Kadam etal .
10. Medicinal chemistry an introduction. By Gareth Thomas.

SEMESTER-III

PROGRAM ELECTIVE-III

3OCPE19.2: 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 catboxylic 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 fermentationexamples. 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 23 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.

Suggested Books

1. Concepts in biotechnology by D. Balasubramananian
2. Principals of biochemistry by Horton.
3. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
4. Chirotechnology: Industrial Synthesis of Optically Active Compound by Roger A. Sheldon

SEMESTER-III

OPEN ELECTIVE-III

3OCOE20.1: 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: Lead modification strategies (12 Hrs)

A. 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.

B. Molecular modeling, Structure and analog based approaches virtual screening, pharmacophore, docking and denovo drug design

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

Introduction to Quantitative-structure–activity relationship studies. QSAR parameters-Pk_a, Hammet constants, LIophilicity constants and Tafts constants. Linear or non-linear relationship between Hammet substituent constant biological activity. Linear or non linear relationship between logp (liophilicity constant) and biological activity. Lipisinki's rule of five multiparameter QSAR-Hansch ananlysis, 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:

a) Hydroxylation: eg. Acetanilide, Nitrazepam, Meprobamate.

b) Reduction: eg. Prontosil, Chloralhydrate.

c) Hydrolysis: eg. Cocaine, Procaine.

d) Oxidation/Reduction: eg. Prostaglandins

e) Conjugations: eg. Glucuronide formation, sulfate formation, acetylation, methylation and conjugation with amino acids.

f) O-Dealkylation and N-Dealkylation: eg. Codeine, Mephobarbital and Chloropromazine.

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

A) Chiral synthesis and Activity of the following Drugs:

S-Ibuprofen, S-Naproxen, Levocetrazine, 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.

Suggested books:

1 Textbook of Organic Medicinal and Pharmaceutical Chemistry by Wilson Gisvold.
2 Medicinal Chemistry by Ashutoshkar.
3 Burger's medicinal chemistry and Drug discovery by Manfred B.Wolf.
4 Introduction to Medicinal chemistry by Graham Patrick.

Further reading:

5 Drug design by E. J. Ariens.
6 Strategies of organic drug design synthesis and design by Daniel Ledneiser.
7 Principles of Medicinal Chemistty by Kadam et al
8 Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
9 Principles of Medicinal Chemistty by Kadam et al

SEMESTER-III

OPEN ELECTIVE-III

3OCOE20.2: 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.

UNTI-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.

Suggested books:

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

Further reading:

1. Principles of Analytical chemistry – M.Valcarcel.
2. R.A Day A.C Underwood Qualitative analysis
3. Handbook of Quality Assurance for the analytical chemistry laboratory, James.P.Dux, Van Nostrand Reinhood, New York, 1986.
4. Training Manuals on ISO 9000 PQM, Giridhar, Raj Publishing House, 2001

SEMESTER-III

LABORATORY-V

3OCL21: ORGANIC CHEMISTRY LAB-II

1. Separation and identification of binary mixtures of organic compounds.
2. Synthesis of organic compounds
   a) Benzillic acid
   b) Benzanilide from Benzophenone
   c) Caprolactam
   d) Vanillyl alchol from vanillin
   e) 2 and 4-Nitrophenol distillation(Nitration and separation by steam distaillation)
   f) O-chloro Benzoic acid from pthallic anhydride.

LABORATORY-VI

3OCL22: SYNTHESIS OF ORGANIC COMPOUNDS AND CHROMATOGRAPHY

1. Laboratory synthesis of the following compounds: 2,5-Dihydroxy acetophenone (Fries reaction), Photo dimerization of maleicanhydride, 4- Nitroacetanilide from acetanilide.

2. Thin layer chromatography: Determination of purity(All the above preparations), monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the Rf values of known standards.

3. Separation/Purification by column chromatography

4. Identification and interpretation of unknown organic compounds by spectra, viz., UV, IR, NMR & mass spectral analysis.

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel.
2. Unitized experiments in organic chemistry by R Q Brewster.
3.Handbook of organic analysis by H T C Clarke.
4.Practical Organic Chemistry by Mann and Saunders.