Rayat Shikshan Sanstha's

Yashavantrao Chavan Institute of Science, Satara (Autonomous)

Department of Chemistry

Syllabus of M. Sc. Part II (Organic Chemistry)

GENERAL OBJECTIVES OF THE COURSE:

1. To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.
2. To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
3. To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, nano science & technology.
4. To conduct lesser written tests and to encourage on non-written tests.
5. To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

Learning Objectives:

1. A graduate with a Master's degree in Chemistry has in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
2. The graduate has expert knowledge of a well-defined area of research within chemistry. The graduate has specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques. Skilled in examining specific phenomena theoretically and/or experimentally, the graduate is able to contribute to the generation of new scientific insights or to the innovation of new applications of chemical research.

STRUCTURE OF COURSE: SEMESTER

Semester	Paper No.	Title	Total Number of lectures/ practical's	Credits
Semester-III	**Theory Course**			
	MCT-301	Organic Reaction Mechanism	60 hrs	4
	MCT-302	Advanced Spectroscopic Methods	60 hrs	4
	MCT-303	Advanced Organic Synthesis	60 hrs	4
	MCT-304	Drugs and Heterocycles	60 hrs	4
	MCT- 305	Theoretical Organic Chemistry	60 hrs	4
	Elective Paper MCT- 305 A	Biomolecular Organic Chemistry	60 hrs	4
	Practical Course			
	MCP-306	Chemistry Practical-V		4
	MCP-307	Chemistry Practical-VI		4
Semester-IV	**Theory Course**			
	MCT-401	Stereochemistry	60 hrs	4
	MCT-402	Chemistry of Natural Products	60 hrs	4
	Elective Paper MCT-402 A	Environmental Chemistry	60 hrs	4
	Practical Course			
	MCP-403	Chemistry Practical-VII		4
	MCP -404	Chemistry Practical-VIII		4
			Total Credits	44

- The semester examination will be conducted at the end of each term (both theory and practical examination)
- Theory paper will be of 80 marks each and 20 marks for internal evaluation test conducted in the mid of the term. Two practicals will be of 100 marks each.
- Question papers will be set in the view of the entire syllabus and preferably covering each unit of the syllabus.

Laboratory Safety Equipment's:

Part: I Personal Precautions:

1. All persons must wear safety Goggles at all times.
2. Must wear Lab Aprons/Lab Jacket and proper shoes.
3. Except in emergency, over – hurried activities is forbidden.
4. Fume cupboard must be used whenever necessary.
5. Eating, Drinking and Smoking in the laboratories strictly forbidden.

Part: II: Use of Safety and Emergency equipment:

1. First aid Kits
2. Sand bucket
3. Fire extinguishers (dry chemical and carbon dioxide extinguishers)
4. Chemical Storage cabinet with proper ventilation
5. Material Safety Data sheets.
6. Management of Local exhaust systems and fume hoods.
7. Sign in register if using instruments

M. Sc. Part – II (Semester – III)

Paper MCT-301: Organic Reaction Mechanism

Learning objectives

i) Distinguish the different of organic reactions mechanisms
ii) Expect reaction products and the changes that occur in the structure of organic compounds interacting depending on the type of interaction.
iii) Expect reaction products according to all mechanisms.
iv) The completion of the shortcomings of a chemical equation by using suitable reagents depending on the type of reactive compound and reaction product.

UNIT-I: Methods of determining reaction mechanism (15)

Kinetic Methods: Order and Molecularity, Methods of following reaction rates, Types of reactions: 1st, 2nd and 3rd order reactions; Reversible, Consecutive and Parallel reactions. Energy of Activation, Entropy of Activation, Effect of Ionic strength,Solvent effect and Kinetic isotopic effect.
Non-Kinetic Methods: Identification of reaction products, Testing of the
possible intermediates, Trapping of the intermediates, Isotopic labeling, Reaction catalysis, Cross-over experiments,Stereochemical studies and Use of physical properties. Hammett and Taft equations.

UNIT–II: Pericyclic reactions (15)

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, classification of pericyclic reaction, Wood-ward Hoffman correlation diagrams,FMO and PMO approach, electrocyclic reactions, conrotatory and disrotatary motions, 4n , 4n+2and allyl systems, cycloaddition, and supra and antara facial additions, 4n and 4n+2 systems, 2+2additions of ketenes, 1,3-dipolar cycloaddition and chelotropic reactions, sigmatropicrearrangement , supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties,(3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

UNIT–III: Name Reactions (15)

A] Mechanism, Stereochemistry, migratory aptitude, (application using complicated example): Dienone –phenol, Favorskii, Baeyer-Villiger, Pinacol- pinacolone, Wolff, Smile's, Mukaiyama esterification, Mitsunobu reaction, Baylis Hillman reaction, Wacker process, Eschenmoser fragmentation, Julia olefination.

B] Protection and deprotection of the following functional groups: hydroxyl, carbonyl, amino and carboxyl with applications

UNIT–IV: Photochemistry (15)

Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photo dissociation gas phase photolysis, photochemistry of alkynes, intermolecular reactions of the olefinic bonds, geometrical isomerism, cyclisation reactions, rearrangements of 1,4 and 1,5-dienes, photochemistry of carbonyl compounds, intramolecular reactions of carbonyl compounds saturated cyclic and acyclic α, β-unsaturated compounds, cyclohexadienones, intermolecular cycloaddition reactions, dimerisation and oxitane formation, photochemistry of aromatic compounds, photo fries

reactions of anilides, photo fries rearrangements. Singlet molecular oxygen reactions, photochemistry of vision.

Learning outcomes

i) Student should understand the difference between kinetic and non-kinetic methods of reaction mechanism.
ii) They must know the exact concept of pericyclic reactions and photochemical reactions.
iii) They must know the Stereochemistry, migratory aptitude of different reactions.

References:

1. A guide book to mechanism in organic chemistry (orient- Longmans)- Peter Sykes [Unit I]
2. Organic Reaction Mechanism (Benjumin)- R. Breslow [Unit I]
3. Mechanism and structure in Organic Chemistry (Holt Reinhartwinston)- B. S. Gould [Unit I]
4. Organic chemistry 1st edition - Clayden, Greeves, Warren, Wothers [All units]
5. Photochemistry and Pericyclic reactions 3rd revised edition, Jagdamba singh and jaya singh
6. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs.
7. Organic reaction mechanism (McGraw Hill) R. K. Bansal
8. Fundamentals of photochemistry K. K. Rohtagi- Mukherji Wiley- Eastern [Unit IV]
9. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
10 Molecular photochemistry, N.J. Urro, W. A. Benjamin [Unit IV]
11. Introductory photochemistry. Cox and T. Camp McGraw –Hill
12. Photochemistry R.P. Kundall and A. Gilbert. Thomson Nelson.
13 Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

M. Sc. Part – II (Semester – III)

Paper MCT-302: Advanced Spectroscopic Methods

Learning objectives

i) Use spectroscopic equipment such as MS, IR, NMR spectrometers.
ii) Identify organic compounds by analysis and interpretation of spectral data.
iii) Explain common terms in NMR (^1H and ^{13}C) spectroscopy such as chemical shift, coupling constant, and anisotropy and describe how they are affected by molecular structure
iv) The ability to investigate and determine the structure of typical organic chemical compounds (molecular weight up to ca. 500) using suitable nuclear magnetic resonance experiments.

UNIT-I: (15)

a) Ultraviolet Spectroscopy (05)

Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of λ max. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls.

b) IR Spectroscopy (10)

Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols; ethers; phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds [ketones; aldehydes; esters; amides; acids; anhydrides; lactones; lactams and conjugated carbonyl

compounds] Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; combination bands and Fermi resonance. FT-IR of gaseous; solids and polymeric materials.

UNIT-II: Mass Spectrometry (15)

Introduction, ion production- EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT-III: NMR Spectroscopy (15)

General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons[aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids;ammines; amides and mercaptons]; chemical exchange; effect of deuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra]; virtual coupling.stereochemistry; hindered rotation; Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique, nuclear overhauser effect [NOE] Resonance of other nuclei. INEPT and INADEQUATE.

UNIT – IV: (15)

a) Carbon-13 NMR Spectroscopy

General considerations; chemical shift [aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compounds]; problems associated with $_{13}C$, FT-NMR, proton decoupled off resonance.

b) Structural problems based on combined spectroscopic techniques (including reaction sequences)

Learning outcomes

i) Student should know the difference in various spectroscopic techniques.
ii) They came to predict the molecular structure of the given problem.
iii) Student should solve the problems by combines spectroscopic entities.

REFERENCE BOOKS:

1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehata) [All units]
2. Donald L. Pavia, Lampman, Kriz, Vyvyan Spectroscop y, Indian edition [All units]
3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCIPY OF ORGANIC MOLECULES (J. Wiley)
4. P.S. Kalsi Spectroscope of organic compounds (New age publisher) [All units]
5. Clayden, Greeves, Warren, Wothers, Organic Chemistry.
6. Jackman and Sterneil , Application of NMR spectroscopy
7. Nuclear magnetic resonance. J.D. Roberts (J. Wiley) [Unit III]
8. Theory and application of U.V. Jafee and Orchin.
9. Mass spectroscopy K. Benjamin. [Unit II]
10. The mass spectra of organic molecules. Beynon J H. [Unit II]
11. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley) [Unit IV]
12. Organic Spectroscopy W. Kemp, ELBS [All units]

M. Sc. Part – II (Semester – III)

Paper MCT-303: Advanced Organic Sythesis

Learning objectives

i) Student should use the logical thinking and imagination for disconnection.
ii) Application of synthetic reagents and metals in organic synthesis.
iii) Implementation of green techniques in synthetic organic chemistry.

UNIT–I: Disconnection approach (15)

An introduction to Synthons and synthetic equivalents, disconnect tion approach, functional group interconversions. One group C-X and two group disconnections in1, 2; 1,3 -1, 4 & 1, 5-difunctional compounds, Retro - synthesis of alkene, acetylenes and aliphatic nitro alcohols and carbonyl compounds, amines. Importance of the Order of events in organic synthesis, Chemoselectivity, Regioselectivity. Protecting groups, Diels-Alder reaction, Michael addition and Robinson annulation. Retro- synthesis of aromatic heterocycles, 3, 4, 5 & 6 membered carbocyclic and heterocyclic rings. Reversal of polarity (Umpolung).

UNIT–II: Application of the reagents and reaction in synthesis. (15)

Complex metal hydrides, sodium cyanoborohydride, lithium diisopropylamide(LDA) Dicyclohexylcarbodiimide(DCC), Trimethylsilyl iodide, peracids, lead tetra acetate, PPA, Diazomethane, ozone, phase transfer catalyst, Woodward-Prevost hydroxylation, Barton and Shapiro reaction, Hoffmann – Loffler-Fretag, Peterson synthesis, Selenium dioxide, Dess-Martin periodinane, periodic acid and iodoisobenzyldiacetate, organ catalysis and Grub's catalysts.

UNIT–III: Applications of metals and non-metals in organic synthesis (15)

Pd, Hg, Cu, Sn, Boron and Si

UNIT–IV: Green chemistry (15)

A] Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. Use of the following in green synthesis with suitable examples: Green reagents: dimethylcarbonate, polymer supported reagents. Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts.

B] Green solvents: Ionic liquids: Synthesis of ionic liquids, applications in alkylation, hydroformylations, expoxidations, synthesis of ethers, Friedel-craft reactions, Diels-Alder reactions, Knoevenagel condensations, Wittig reactions, Phase transfer catalyst, Synthesis, applications.

C] Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions. Ultrasound assisted reactions. Comparison of traditional processes versus green processes in the syntheses.

Learning outcomes

i) Student should able to predict the designing of molecule with correct disconnection.
ii) Students are skilled in reaction mechanism of different synthetic reagents and metals.
iii) Students are skilled to perform green synthetic procedure like microwave, ultrasonic bath, as well as different green solvents like ionic liquids, DEM, etc.

REFERENCE BOOKS:

1. Designing of organic synthesis.S.Warren [Unit I]
2. Organic synthesis J. Fuhrhop& G. Penzlin. (2nd ed.)
3. Some modern methods of organic synthesis.Carruthres: [Unit II, III]
4. Modern synthetic reaction.H.O.House [Unit II, III]
5. Reagent in organic synthesis. Fieser&Fieser [Unit II, III]
6. Principle of organic synthesis. R.O.C.Norman [Unit II, III]
7. Advanced organic Chemistry. Carey&Sundharg
8. Organic synthesis. P.E.Realand: [Unit IV]
9. Comprehensive organic Chemistry. Bartan and Ollis :
10. Organic reactions.R.Admas
11. Advances in organometallic Chemistry. Stone & West [Unit III]

M. Sc. Part – II (Semester – III)

Paper MCT-304: Drugs and Heterocycles

Learning objective

i) Computational approach in designing of a molecule.
ii) Conceptual leaning of drug discovery.
iii) Synthesis of five, six, membered etc heterocycles with mechanistic approach.

UNIT–I: Drug discovery and design (15)

Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs. Theories of drug activity, Quantitative structure activity relationship. Theories of drug ctivity, Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors.

(B) Computational Chemistry

Introduction, applications in organic synthesis and its role in drug dievery.

UNIT–II: Synthesis of drugs (15)

(A)Study of Antibiotics

Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, general account of tetracycline & macrocyclic antibiotics (no synthesis).

(B) Synthesis

a) Antimalerials: Trimethoprim.

b) Analgesic & Antipyretics: Paracetamol, Meperidine, methadone, Aminopyrine.
c) Anti- inflammatory: Oxyphenylbutazone, Diclophenac, Indomethacin.
d) Antitubercular & antileprotic: Dapsone
e) Anaesthetics : Lidocaine, Thiopental.
f) Antihistamines: Diphenylhydramine.
g) Tranquilizers: Diazepam, Trimeprazine.
h) Anti AIDS: General study
i) Cardiovascular: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol.
j) Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards. Recent development in cancer chemotherapy. Hormones and natural products.

UNIT–III: Heterocyclic Chemistry-I (15)

a) Five and six membered heterocycles with one and two hetero atoms:
Synthesis, reactivity, aromatic character and importance of following heterocyclic rings: Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, Pyridine, Pyrimidine, diazines

b) Five and Six membered Heterocycles with more than two Heteroatoms
Synthesis and reactions of triazines, 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole.

UNIT – IV: Heterocyclic Chemistry-II (15)

a) Benzofused Heterocycles
Synthesis and reactions of benzopyrroles, benzofurans, benzothiophenes, Benzoxazole, Benzthiazole, and Quinoline, Benzimidazole

b) Six membered Heterocycles with one heteroatom
Synthesis and reactions of pyrilium salts and pyrones and their comparison pyridinium
And thiopyrylium salts and pyridones. Synthesis and reactions of coumarins, chromones.

Learning outcomes

i) Student studied the drug synthesis with their computational designing.
ii) Student studied the different heterocyclic systems: Generation and their synthetic application.

REFERENCE BOOKS:
1. Medicinal Chemistry.Burger : [Unit I, II]
2. Medicinal Chemistry A. Kar. (Wiley East) [Unit I, II]
3 Principals of medicinal chemistry.W. O. Foye : [Unit I, II]
4 Text book of organic medical and pharmaceuticalchemistry. Wilson, Gisvold&Dorque: [Unit I, II]
5 Pharmaceutical manufacturing encyclopedia.
6 An introduction to chemistry of heterocyclic compounds.R. M. Acheson:(Interscience).
7 Heterocyclic chemistry. Joule &Smith : (Van Nostrand). [Unit III, IV]
8 Heterocyclic chemistry. R. K. Bansal: (Wiley E). [Unit III, IV]
9 Principals of modern heterocyclic chemistry.L. A. Paquitte :
10 The structure and reactions of heterocyclic compounds.M. H. Palamer : [Unit III, IV]
11 Advances in Heterocyclic chemistry. A. R. Katritzky: (A.P.). [Unit III, IV]

12 Organic chemistry (Vol. 1& 2)Finar.
13 Outline of Biochemistry.Cohn &Stumpt
14 Introduction to the chemistry of enzyme action.Williams :
15 The Organic Chemistry of Drug design and Drug action. R. B. Silverman Academic press.
16 Strategies for Organic Drug synthesis and Design. D. Lednicer, J. Willey. [Unit I, II]
17 Heterocyclic Chemistry. Vol-1-3, R. R. Gupta, M. Kumar and V. Gupta, [Unit III, IV] SpringerVeriag.

M. Sc. Part – II (Semester – III)

Paper MCT-305: Theoretical Organic Chemistry

Learning objective

i) Able to absorb the aromaticity concept of non-benzoid system.
ii) Student must know the supramolecular chemistry with various molecules.
iii) Able to know the difference between the kinetic and thermodynamic controlled reactions with applications

UNIT–I: Molecular Orbital Theory (15)

Aromaticity in benzenoids, alternant and non alternant hydrocarbon, Huckels rule, energy level of pi- molecular orbital and concept of aromaticity, calculation of energies of orbitals cyclic and acyclic systems. Determination energies and stabilities of different systems calculation of charge densities PMO theory and reactivity index.

UNIT – II: Supramolecular Chemistry (15)

Host-Guest approach, Chiral recognition, Ionophores, Crown ethers, cryptands, Micelles, Cyclodextrins, calixarenes. Annulenes and heteroannulenes, fullerence C60, tropone, tropoloneazulene, fulvene, tropylium salts, ferrocene, Three and five membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes and rotaxanes, bonding in fullerenes.

UNIT – III: Free radical reactions (15)

Types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance. Reactivity for aliphatic and aromatic ubstrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction. Free radical rearrangement, Hunsdiecker reaction.

UNIT – IV (15)

a) Kinetic and thermodynamic control of reactions (9)

Nitration and Sulphonation of naphthalene, Wittig, Enolization, Friedel-Crafts and Diels Alder reactions.

b) Non-classical carbocations: Formation, stability and reactivity**. (6)**

Learning outcomes

i) Student should understand the MOT and the concept of aromaticity.
ii) They must know the free radical reactions, kinetic and thermodynamic controlled reactions.
iii) They should the know the supramolecules with their structural explanation.

REFERENCE BOOKS :

1. 1.Lehar and Merchand: Orbital Symmetry. [Unit I, II]
2. R. B. Woodward and Hoffman: Conservation of orbital symmetry.
3. Kan: Organic Photochemistry
4. Cixon and Halton : Organic photochemistry
5. Arnold: Photochemistry
6. N. Turro : Modern molecular photochemistry.
8. Ginsburg: Nonbenzenoid aromatic compound. [Unit III, IV]
9. A. Streitwieser : Molecular orbital theory for organic chemistry.
10. E. Cler : The aromatic sextet. [Unit II]
11. Lloyd: Carbocyclic non- benzenoid aromatic compounds. [Unit I]
12. W. B. Smith: Molecular orbital methods in organic chemistry.

Elective Paper

M. Sc. Part – II (Semester – III)

Paper MCT-305 A: BIMOLECULAR ORGANIC CHEMISTRY

Learning objective

i) Discuss similarities and differences between transformation of biomolecules in living systems.
ii) Describe various biomolecles which are important in living organisms.
iii) Corelate the chemical structure of biomolecles to reactivity.

UNIT–I: Amino acids, peptides and proteins (15)

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure.Tertiary structure of protein: folding and domain structure. Quaternary structure. Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation. Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, Phosphoramidite and H-phosphonate methods including solid phase approach. Computational study of proteins.

Unit II: Enzymes (15)

Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: i) Enzyme efficiency/catalytic power ii) Enzyme

specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site.Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond.

Unit-III: Organic Smart Materials (15)

Introduction, shape memory material (SMM) and shape memory technology (SMT), types of smart materials: Piezoelectric, Shape-memory alloys and shape-memory polymers, Photovoltaic materials or optoelectronics, Electroactive polymers (EAPs), Magnetostrictive, Smart inorganic polymers,Temperature-responsive polymers, Halochromic materials, Chromogenic systems, thermochromic materials, Ferrofluids ,Photomechanical materials, Polycaprolactone (polymorph),Self-healing materials, Magnetocaloric materials, Thermoelectric materials, Chemoresponsive materials. Classification of photomechanical organiccrystals based on photo reactions. Applications

UNIT–IV: Lipids (15)

Fatty acids, essential fatty acids, structures and function of triglycerides, glycerophspholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteinscomposition and function, role in arthrosclerosis. Properties of lipid aggregates – micelles, bilayers, liposomes and their possible biological functions. Biological members .Fluid mosaic model of membrane structure. Lipid metabolism - β-oxidation of fatty acids

Learning outcomes

i) Student should learn about the reactivity and applications of biomolecles.
ii) They must know about the different bimolecular organic molecules and their role in living systems.
iii) Student will understand the outlines of biochemical reactions.

REFERENCE BOOKS:

1. Principles of Biochemistry, A. L. Lehinger, Worth Publications. [Unit I]
2. Biochemistry, L. Stryer, W. H. Freeman [Unit I, II]
3. Biochemistry, J. David Rawn, Neil Patterson. [Unit I, II]
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.

Practical Course (Paper MCP-306 & 307)

M.Sc. Part-II (Sem-III)
MCP 306 & 307 Organic Chemistry Practical

A. Qualitative Analysis

Separation, purification and identification of compounds of ternary mixtures using semi microanalysis, TLC, column chromatography and chemical tests. IR spectra to be used for functional group identification. Assign therotical value of ^{1}H NMR, ^{13}C NMR and Mass Spectroscopy of chemical compounds of ternary mixture.

B. Analysis of commercial available active organic compound and its comparison with natural compounds which is extracted from natural sources.

C. Quantitative analysis

1. Two step Preparations (Any Three)

1. Benzaldehyde → Benzalacetophenone → Epoxide
2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid
3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin
4. Cyclohexanone → Phenyl hydrazone → 1,2,3,4-Tetrahydrocarbazole
5. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene
6. Acetanilide → p-Acetamidobenzene sulphonyl chloride → P. Acetamidobenzene sulphonamide
7. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetanilide
8. Hippuric acid → Azalactone → 4-Benzylidene 2-phenyl oxazol-5-one
9. p-Cresol → p-Cresyl benzoate → 2-Hydroxy-5-methyl benzophenone
10. Phthalimide → N-Benzylphthalimide → Benzylamine
11. o-Nitroaniline → o-Phenylene diamine → Benzimidazole
12. Phthalic acid → Phthalimide → Anthranilic acid
13. Benzyl cyanide→ p-Nitrobenzyl cyanide→p-Nitro phenyl acetic acid
14. Hydroquinone → Hydroquinone diacetate → 2,5-Dihydroxy acetopheneone
15. Cyclohexanone→ Enamine→2-Acetyl cyclohexanone
16. α-Pinene→ Disiamyl borane→Pinanol
17) Preparation of m-Nitroaniline
18) Preparation of Benzanilide from benzophenone
19) Preparation of Phthalimide
20) Preparation of N-Bromosuccinimide
21) Benzilic acid rearrangement: Benzilic acid from benzil
22) Sandmeyer reaction: p-Nitroiodobenzene from p-nitroaniline
23) Heterocyclic compound: 7-Hydroxy-4-methylcoumarin from resorcinol
24) Acetylation: Mannitol hexaacetate from mannitol
25) Claisen-Schmidt reaction: Dibenzalacetone from benzaldehyde
26) Oxidation: Fluorenone from fluorene
27) Acetylation: Acetylferrocene from ferrocene
28) Synthesis of acetanilide from aniline.

2. Structure elucidation by using given spectral data as well as perform its retrosynthetic analysis.

3. Any other suitable expt. may be added

Learning Outcomes

1) Student should understand the difference between water soluble and ether soluble components.
2) Student must know the separation method of ternary mixture by mirco technique (Green approach).
3) Student should understand two step preparations of different reactions.
4) Student should understand how and why to check TLC for monitoring the reaction.

5) Student should understand the method of solving spectral problems by spectra of different compounds

RECOMMONDED BOOKS:

1. Textbook of Practical Organic Chemistry – A. I. Vogel.
2. Practical Organic Chemistry – Mann & Saunders.
3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
4. Organic Synthesis Collective Volumes by Blat

M. Sc. Part – II (Semester – IV)

Paper MCT-401: Stereochemistry

Learning objectives

i) How to implement the newer methods of stereoselective synthesis?
ii) Student able to implement the conformational approach to acyclic and alicyclic systems.
iii) They able to learn the advanced stereochemistry with some advanced knowledge such as crams rule, Felkin Ahn rule, Octant rule, etc.

UNIT- I: Newer methods of stereoselective synthesis. (15)

Introduction and Stereoselective and Stereospecific reactions; Enantioselective synthesis (chiral approach) reactions with hydride donors, hydroboration, catalytic hydrogenation via chiral hydrazones and oxazolines, Sharpless epoxidation, Diels Alder selective synthesis, Aldol and related reactions including Cram's rule and Felkin Anh rule use of calculations of optical purity and enantiomeric excess.

UNIT- II: Stereochemistry of acyclic and alicyclic compounds (15)

A) Conformation and reactivity in acyclic compounds and of cyclohexanes. **(5)**
Stability and Reactivity of diastereoisomers. **Curtin- Hammett principle**.

B) Some aspects of the stereochemistry of ring systems: (**5**)
Stereoisomerism and determination of the configuration of alicyclic rings; Stability of rings and ease of rings formation

C) The shapes of the rings other than six membered: **(5)**
Shapes of five, six, and seven membered rings. Conformational effects In medium sized rings, Concept of' I'strain.

UNIT-III: Stereochemistry of the ring system, conformation and configuration (15)

a) Fused and bridged rings: Fused bicyclic ring systems: **(8)**
Types of fused ring systems, Cis and trans-Decalins, Perhydroanthracene, Perhydrophenanthrene; **Bridged rings**: Types of bridged ring systems, Nomenclature, stereochemical restrictions, and Bredt's rule.

b) O.R.D. and C.D.: Types of curves, circular dichroism**,** Determination of the conformation and configuration, The Octant rule and axial haloketone rule. **(7)**

UNIT-IV: Stereochemistry of compounds containing no chiral carbon atoms and diastereoisomerism (Geometrical isomerism) (15)

a) Stereochemistry of Allenes, Spiranes and Biphenyls **(8)**
Assignment of configuration

b) Configuration of diastereomers (Geometrical isomerism) based on physical and chemical methods**.** **(7)**

Learning outcomes

i) Student should understand difference between basic stereochemistry and modern stereochemistry.
ii) Student must explore conceptual fact of stereoselective synthesis.
iii) Student should understand the shapes of ring other than five membered.
iv) Student must learn the allene, spirane and biphenyls systems.

REFERENCE BOOKS:

1. E.L. Eliel : Stereochemistry of carbon compounds. [All units]
2. D. Nasipuri : Stereochemistry of organic compounds [All units]
3. P.S. Kalsi: Stereochemistry, Conformation and Mechanism. [All units]
4. Eliel, Allinger, Angyal and Morrison : Conformational analysis.
5. Hallas: Organic stereochemistry
6. Mislow and Benjamin: Introduction to Stereochemistry.
7. H. Kagan : Organic stereochemistry.
8. Carl Djerassi ; Optical Rotatory Dispersion. [Unit III]
9. P. Crabbe : Optical Rotatory Dispersion and C.D. [Unit III]

M. Sc. Part – II (Semester – IV)

Paper MCT-402: Chemistry of Natural Products

Learning objectives

i) Introduction of naturally occurring organic molecules.
ii) Synthesis of heavily substituted molecules like steroids, terpenoids, prostaglandins, etc.
iii) Designing a natural product through a biogenesis approach.

UNIT-I: a) Introduction of natural products **(3)**
Classification and isolation methods.

b) Terpenoids **(12)**
Introduction of natural products : Classification and isolation methods
carvone, abietic acid, zingiberene, α-santonin, β-cuparenone and β-caryophyllene.

UNIT-II: Alkaloids **(15)**
Structure, stereochemistry, synthesis and biosynthesis of the following: Morphine, Reserpine,

UNIT-III: a) Steroids **(10)**

Occurrence, nomenclature, basic skeleton, Diels hydrocarbon. **Study of the following**: hormones, Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and cortisone (only synthesis).

b) Prostaglandins **(5)**

Occurrence, nomenclature, classification, biogenesis and physiological effects, Synthesis of PGE2 and PGE2

UNIT-IV: a) Biogenesis **(8)**

a) **Terpenoids** :mono, sesqui.,, di- and triterpenoids, cholesterol.
b) **Alkoloids** : Derived from ornithine, lysine, tyrosine, tryptophan, pyridine, morphine and indole type alkoloids.
c) **Shikimatefathway** – cinnamic acids, lignans, coumarins, flavonoids, isoflavonoids and terpenoids quinines and the compds. belonging to the classes bisabolene, eudesman and steroids,cholesterol, steroids.

b) Vitamins **(7)**

Synthesis and structure of **biotin** and vitamin **B_1, B_2, B6: biological** functions of Vitamin**B_6**,**D** and **E**.

Learning outcomes

i) Student should understand Classification and isolation methods.
ii) Student should know Structure and synthesis of camphor, carvone, abietic acid, zingiberene, α-santonin, β-cuparenone and β- caryophyllene.
iii) Student should understand different Structure, stereochemistry, synthesis and biosynthesis the following: Morphine, Reserpine, Ephedrine and (+) Conin.
iv) They should understand Occurrence, nomenclature, classification, biogenesis and physiological effects, Synthesis of PGE2 and PGE2

REFERENCE BOOKS:

1. Apsimon: The total synthesis of natural products.
2. Manskey and Holmes: Alkaloids
3. A.A. Newmen: Chemistry of Terpenes.
4. P. D B.Mayo: The chemistry of natural products.
5. Simonson: Terpenes. [Unit I]
6. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry.
7. Woguer: Vitamins and Co- enzymes.
8. P. W. Bently: Chemistry of Natural products,
9. Fieser and Fieser: Steriods [Unit III]
10. I. Finar: Organic chemistry Vol. II and I [All units]
11. J.B. Hendrickson, The molecules of nature.
12. Peter Bernfield: The biogenesis of natural products [Unit IV]
13. R.T. Slickenstaff A.C. Ghosh and G.C. Wole : Total synthesis of steroids.
14. The chemistry of natural products, vol. Nakanishi.

Elective Paper

M. Sc. Part – II (Semester – IV)

Paper MCT-402 A: Environmental Chemistry

Learning objectives

i) To provide students with broad theoretical and applied background
ii) To provide basic principles of basic principles of environmental chemistry.
iii) To give idea about collection of data regarding chemical and biological in relation with environment.
iv) Student will know environmental problems relating to society.

UNIT-I: Introduction to Environmental Chemistry **[15]**

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

UNIT-II: Atmosphere, Hydrosphere and Lithosphere **[15]**

Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer. Hydrosphere: Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions. Lithosphere: Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

UNIT-III: Chemical Toxicology **[15]**

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

UNIT-IV: **[15]**

A) Air Pollution

Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, Photochemical smog, Air-quality standards

B) Water Pollution and water treatment

Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Learning outcomes

i) Student getting idea about basic principles of environmental chemistry
ii) Student understands the environmental issues regarding social aspects.
iii) Student meets the burning issues of environment with their remedies.

Reference Books:

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, Oxford University

Press (2000).
2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
3. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).
4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd.,New Delhi. [All units]
5. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York. [All units]
6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi. [All units]
7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

Practical Course (MCP-403 & 404)

M.Sc. Part-II (Sem-IV)
MCP 403 & 404 Organic Chemistry Practical Course VII and VIII

1. Estimation of Sulphur and Nitrogen.

2. Three stage organic preparations
1. Preparation of Anthranilic acid.
2.Preparatin of p- Amino benzoic acid.
3.Preparation of p- Chloro nitrobenzene by Sandmeyer reaction.
4.Preparation of p- Iodonitrobenzene by Sandmeyer reaction.
5.Multicomponent synthesis.

Green methods of synthesis (Microwave and ultrasonic technique)
1. Synthesis of Schiff's base from aniline and p-anisaldehyde in the presence of lime juice
2. Synthesis of coumarin by Knoevenagel reaction using salicylaldehyde, and ethyl acetate in presence of a base.
3. Synthesis of dihydropyrimidones- Biginelli reaction: acid-catalyzed three component reaction between vanillin, ethyl acetoacetate and thiourea.
4. Synthesis of acetanilide from aniline.

3. Project: Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, use of new methods etc. Identification of organic compounds by spectroscopic methods. External and internal examiners will examine the project (50 Marks) jointly at the time of practical examination.

4. Any other suitable experiments may be added.

Learning Outcomes

1) Student should understand the three step preparations.
2) Student must know the method of estimation of sulfur and nitrogen.
3) Student should understand how to assemble Kjeldahl's apparatus for estimation of nitrogen.
4) Student should understand Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products.

5) Student should understand standardization of reaction conditions, use of new methods etc. Identification of organic compounds by spectroscopic methods

RECOMMONDED BOOKS:

1. Textbook of Practical Organic Chemistry – A. I. Vogel.
2. Practical Organic Chemistry – Mann & Saunders.
3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
4. Organic Synthesis Collective Volumes by Blat