SEMESTER-III

PAPER I - ORGANIC REACTION MECHANISMS, PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

(Effective from the admitted batch of 2023-2024)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of radical reactions and mechanisms of Substitution and their importance.
CO 2: Understand the concept of mechanisms of Pericyclic reactions
CO 3: Understand the advanced reactions and mechanisms of Pericyclic reactions
CO 4: Develop interest in the areas of reactions and mechanisms of Organic Photochemistry
CO 5: Develop concepts of advanced reactions and mechanisms in Organic Photochemistry

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Familiarize the different types of nucleophilic and radical substitution reactions
LO 2: Analyze and solve to add nucleophiles, electrophiles and free radicals to carbon-hetero atom multiple bonds
LO 3: Interpret theoretical basis of pericyclic reactions and helps them to carry out these reactions.
LO 4: Apply the concept of pericyclic reaction in synthesis of organic compounds
LO 5: Basic concepts of organic photochemical reactions
LO 6: Photochemistry of carbonyl compounds, alkenes, dienes and aromatic compounds
LO 7: To know synthetically the processes relevant organic-chemical reactions and be able to discuss the mechanism of these reactions

UNIT-I: Radical Substitution Reactions **[12 Hours]**

Reactivity for aliphatic substrates, reactivity at Bridgehead, Reactivity in aromatic substrates, neighbouring group assistance in free radical reactions, reactivity in the attacking radical, effect of solvent on reactivity, halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, Hunsdiecker reaction, Kolbe reaction, Reed reaction and Sandmayer reaction.

UNIT-II: Pericyclic reactions-I: **[12 Hours]**

Molecular orbital symmetry - frontier orbitals of ethylene - 1,3-Butadiene, 1,3,5-Hexatriene, allyl system - classification of pericylic reactions - FMO approach - Woodward-Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions. **Electrocyclic Reactions:** Conrotatory and disrotatory motions, (4n) and (4n+2) - allyl systems and secondary effects. **Cycloadditions:** Antarafacial and suprafacial additions, notation of cycloadditions, (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+2) - cycloadditions, and cheletropic reactions.

UNIT-III: Pericyclic reactions-II: [12 Hours]

FMO approach and perturbation of molecular (PMO) approach for the explanation of sigmatropic rearrangements under thermal and photochemical conditions - suprafacial and antarafacial shifts of H - sigmatropic shifts involving carbon moieties - retention and inversion of configurations, (3,3) and (5,5) sigmatropic rearrangements - detailed studies of Claisen (Ireland-Claisen, Overman-Claisen, Johnson-Claisen) and Cope rearrangements - aza-Cope rearrangement and fluxional tautomerism

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UNIT-IV: Organic Photochemistry-I: [12 Hours]

Photochemical energy, Frank-Condon Principle - Jablonski diagram singlet and triplet states - dissipation of photochemical energy – photosensitization – quenching - quantum efficiency and quantum yield - experimental methods of photochemistry - photochemistry of carbonyl compounds n-π, π-π* transitions - Norrish type I and Norrish type II cleavages - Paterno-Buchi reaction.

UNIT-V: Organic Photochemistry-II: [12 Hours]

Photo reduction - hydrogen abstraction - rearrangement of α,β- unsaturated ketones and cyclohexadienones - photochemistry of p-benzoquinones - photochemistry of unsaturated systems – olefins, *cis-trans*-isomerization and dimerisation - hydrogen abstractions and addition acetylenes dimerization, dienes - photochemistry of 1,3-butadiene - photochemistry of cyclohexadienes. Di-pi methane rearrangement

Photochemistry of aromatic compounds – excited state of benzene and its 1,2-, 1,3-, 1-4- additions - photofries rearrangement - photofries reactions of anilides, photosubstitution reactions of benzene derivatives.

Text Books:

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
2. Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
3. Pericyclic reactions by S.N. Mukharji, Mcmilan.
4. Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Richgardson.
5. The modern structural theory in Organic Chemistry by L.N.Ferguson, Pretice Hall.

GAYATRI VIDYA PARISHAD COLLEGE FOR DEGREE AND PG COURSES (A)
DEPARTMENT OF ORGANIC CHEMISTRY
M.Sc. (Final) CHEMISTRY SYLLABUS
SEMESTER-III, PAPER-II- ORGANIC SPECTROSCOPY
(Effective from the admitted batch of 2023-2024)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the in-depth knowledge on UV Spectroscopic technique.
CO 2: Acquire the in-depth knowledge on IR Spectroscopic technique.
CO 3: Acquire the in-depth knowledge on NMR Spectroscopic technique. Understand the concepts like Chemical shifts, spin-spin splitting
CO 4: Acquire the in-depth knowledge on Mass Spectroscopic technique. Understand the concepts of fragmentation process
CO 5: Develop and apply interest in the areas of UV, Infrared, NMR and Mass Spectroscopic techniques and structural elucidation of organic compounds using the data obtained

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain the concept of UV spectroscopic techniques and interpret the values of dienes, dienophiles and aromatic compounds.
LO 2: Analyze the spectral data using IR spectroscopy
LO 3: Interpret the structure of different organic molecules using NMR spectroscopy
LO 4: Apply the concept of spin-spin splitting, coupling constants for different organic compounds for data interpretation.
LO 5: Identify the organic molecules using Mass spectroscopy
LO 6: Elucidate structure of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.

UNIT-I: UV SPECTROSCOPY: **[12 Hours]**

UV spectra of aromatic and heterocyclic compounds, α-diketones, β-diketones, enediones and quinines. Applications of UV Spectroscopy-study of isomerism, determination of strength of hydrogen bonding.

UNIT-II: Infrared Spectroscopy: **[12 Hours]**

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, carboxylic acids, anhydrides, lactones, lactums, nitriles and conjugated carbonyl compounds. Effect of hydrogen bonding and solvent on vibrational frequencies.

UNIT-III: Nuclear Magnetic Resonance Spectroscopy (1H NMR):[12 Hours]

Nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shifts and its measurements, factors affecting chemical shift, chemical and magnetic equivalence of spins, spin-spin coupling, integration, the coupling constant, types of spin-spin couplings, factors influencing coupling constants, first-order and non-first order spectra, spin system notations (ABX, AMX, ABC, A_2B_2 etc.). Simplification of non-first order spectra- use of higher magnetic fields, Deuterium exchange, Nuclear Overhauser Effect difference spectra,

UNIT-IV: Mass spectroscopy: **[12 Hours]**
McLafferty rearrangement, ortho effect. *retro*-Diels-Alder reaction, Fragmentation processes- fragmentation associated with various functional groups (alkanes, cycloalkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amides, amines, alkyl chlorides and alkyl bromides.

UNIT-V: Application of UV, IR, NMR and MASS **[12 Hours]**
Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.

Textbooks:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
2. Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-Ur-Rahman

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SEMESTER-III, PAPER-III-ORGANIC SYNTHESIS
(Effective from the admitted batch of 2023-2024)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of formation of C-C using various reagents.
CO 2: Acquire the knowledge of formation of C=C using various reagents.
CO 3: Develop knowledge on various Oxidizing reagents used in organic synthesis
CO 4: Develop knowledge on various reducing reagents used in organic synthesis
CO 5: Develop interest in the areas of Asymmetric Synthesis

Course learning outcome (LOs):

Upon completion of the course the students should be able to:
LO 1: Apply the concept of C-C bond formation using various reagents in organic synthesis.
LO 2: Apply the concept of C=C bond formation using various reagents in organic synthesis.
LO 3: Apply different oxidizing reagents in organic synthesis
LO 4: Apply different reducing reagents in organic synthesis
LO 5: Explain and apply the knowledge of asymmetric synthesis in synthesizing pure enantiomers
LO 6: apply formation of C-C and C=C bonds, organic polymers, unactivated C-H bonds, Asymmetric Synthesis

UNIT-I: Formation of Carbon-Carbon (C-C) single bonds: [12 Hours]

Alkylations *via* enolate - the enamine and related reactions - umploung (dipole inversion) – the aldol reaction – applications of organopalladium (Heck-Suzuki coupling and Stille-Sonogishira cross coupling - Negishi-Kumada coupling reactions) and organocopper reagents (Gillman reagent) - applications of sulphur ylides - synthetic applications of carbenes and carbenoids.

UNIT-II: Formation of carbon-carbon double bonds: **[12 Hours]**

Elimination reactions – pyrolytic syn eliminations – sulphoxide -sulphonate rearrangement - Wittig reaction-alkenes from arylsulphonylhydrazones (Shapiro reaction) - Eschenmoser fragmentation - olefin metathesis (Grubb's reaction), Peterson's olefination.

UNIT-III: Oxidation [12 Hours]

Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium, DMSO, and TEMPO based reagents). (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. (d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, and ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (selenium, chromium based allylic oxidation)

UNIT-IV: Reduction **[12 Hours]**

Reduction:(a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium/Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and (Birch, Pinacol formation, McMurry, Acyloin formation, dehalgenation and deoxygenations) (c) Hydride transfer reagents-NaBH4 triacetoxyborohydride, L-selectride, K-selectride; LiAlH4, DIBAL-H, and Red-Al.

UNIT-V: A) Asymmetric Synthesis **[12 Hours]**

Topocity – Prochirality – Substrate selectivity – Diastereoselectivity and enantioselectivity –Substrate controlled methods – use of chiral substrates – examples Auxiliary controlled methods – Use of chiral auxiliaries – Chiral enolates – alkylation of chiral imines-Reagent controlled methods – Use of chiral reagents – Asymmetric oxidation – Sharpless epoxidation – Asymmetric reduction – borate reagents.

Text Books:

1. Some Modem Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. BenzamineInc. Menio Park, California, 1972.
3. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon. (ELBS)
4. Advanced organic chemistry part A & B; Fourth edition; Francis A Cary and Richard J. Sundberg; Kluwer Academic/Plenum Publisher New York, 2000.
5. Organic chemistry Jonathan Clayden, Nick Geeves, Stuart Warren, 2nd Edition, 2012, Oxford University Press.
6. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri.
7. Stereochemistry of Carbon compounds by Ernest L Eliel& Samuel H. wilen.
8. Stereochemistry: Conformation & Mechanism by P S Kalsi.
9. The third dimension in organic chemistry, by Alan Bassendale.
10. Stereo selectivity in organic synthesis by R S Ward.
11. Asymmetric synthesis by Nogradi.
12. Asymmetric organic reactions by J D Morrison and H S Moschcr.
13. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE.

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SEMESTER-III, PAPER-IV-CHEMISTRY OF NATURAL PRODUCTS
(Effective from the admitted batch of 2023-2024)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 60	Internal: 40

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, Acetogenins and shikimates

CO 2: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected terpenes

CO 3: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected steroids.

CO 4: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected alkaloids

CO 5: Acquire the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of amino acids, proteins and nucleic acids

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Explain the isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected antibiotics, Acetogenins and shikimates

LO 2: Apply the knowledge of isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected terpenes

LO 3: Develop the interest in isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected steroids.

LO 4: Develop the interest in isolation, structural elucidation, stereochemistry, synthesis and biological properties of selected alkaloids

LO 5: Explain the isolation, structural elucidation, stereochemistry, synthesis and biological properties of amino acids, proteins and nucleic acids

LO 6: apply the knowledge of structure, isolation and synthesis of various natural products to develop new derivatives.

UNIT-I: **[12 Hours]**

A) Antibiotics **:** Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Penicillin G, Cephalosporin-C.

B) **Acetogenins and shikimates:** Prostaglandin 15 R PGA_2 - podophyllotoxin - etoposide

UNIT-II:
Terpenes **[12 Hours]**
Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Terpenes: Forskolin, Taxol and Azadirachtin

UNIT-III: **[12 Hours]**
Steroids: Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Steroids: Cholesterol - progesterone – testosterone

UNIT-IV:
Alkaloids **[12 Hours]**
Isolation, structure elucidation, stereochemistry, synthesis, and biological properties of Alkaloids: Morphine, camptothecin.and Vincristine

UNIT-V: **[12 Hours]**
A) Peptides and Proteins: α-Aminoacids, their general properties and synthesis, Synthesis of peptides by Merrifield solid phase synthesis. Primary, secondary and tertiary structures of proteins
B) Nucleic acids: Heterocyclic bases; Purines: Adenine and Guanine; Pyramidines: Cytosine, Uracil and Thymine; nucleosides, nucleotides Basic concepts of the structures of RNA and DNA

Text Books:

1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of natural products, I.L. Finar, 5th Edition. ELBS.
2. Chemical A spects of Biosynthesis, John Mann, Oxford University Press, Oxford,1996
3. Chemistry of Natural Products. A Unified Approach, N.R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
4. Chemistry of Natural Products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010.

P. Uma Devi

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VISAKHAPATNAM

DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. (Final) ORGANIC CHEMISTRY PRACTICALS
SEMESTER-III
(Effective from 2023-2024 admitted batch)

Credits: 8		Theory: 15 Hours
Max Marks: 200	External: 160	Internal: 40

PRACTICAL SYLLABUS

Practical I
Multistage synthesis of six organic compounds involving three or more stages.

Practical II
1. Thin Layer Chromatography
2. Column Chromatography

Text Books:

1. Vogel's Practical Organic Chemistry, A.R. Tatchell, B.S. Furnis, A.J. Hannaford and P.W.G. Smith, 5th Edition, Pearson, New Delhi, 2017.

2. Vogel's Text book of Quantitative Inorganic Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th Edition, Pearson Education, New Delhi, 2008.

3. Chemistry of Natural Products: A Laboratory Handbook, N.R. Krishnaswamy, Universities Press, Hyderabad, 2013.

4. A Laboratory Manual of Organic Chemistry, R.K. Bansal, New Age International Publishers, New Delhi, 2008.

5. Practical Organic Chemistry, F.G. Mann & B.C. Saunders, Pearson, New Delhi, 2001.

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