



Anekant Education Society's

**Tuljaram Chaturchand College
of Arts, Science, Commerce, Baramati**

(Autonomous)

DEPARTMENT OF CHEMISTRY

(Faculty of Science and Technology)

Two Year MSc Degree Program Chemistry

MSc. II Organic Chemistry

(2019 Pattern)

Choice Based Credit System Structure and Syllabus

(To be implemented from June 2019)

M.Sc.-II Organic Chemistry
(2019 Pattern)
Semester – III
CHO-5301: Designing of organic synthesis and Heterocyclic Chemistry
(48 L+ 12 T) (4 Credit)

Course Objective: On completion of the course, the student will be able to:

- 1) To provide students with a thorough understanding of the principles and strategies involved in retrosynthetic analysis, including the identification of key functional groups, disconnections, and the selection of appropriate synthetic pathways.
- 2) To introduce students to the concept of protecting functional groups during organic synthesis and the selection of appropriate protective groups.
- 3) To provide students with a solid foundation in the principles and concepts of heterocyclic chemistry, including the classification, nomenclature, and synthesis of heterocyclic compounds.
- 4) To explore the reactivity patterns of different heterocyclic systems and their synthetic methods, including both traditional and modern approaches.
- 5) To enhance students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze and solve complex problems related to heterocyclic chemistry.
- 6) To develop students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze complex synthetic problems, propose synthetic routes, and evaluate the feasibility and efficiency of different strategies.
- 7) To understand the rationale behind protection, the methods for introducing and removing protective groups, and the impact of protective groups on reaction selectivity.

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis.
- CO2. Expertise in reactions using protection and deprotection methods.
- CO3. Demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.
- CO4. Describe methods for synthesis and transformation of the most common functional groups
- CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
- CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

1. Designing of organic synthesis (24 L)

Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide, enamines, Umpolung inorganic synthesis, Retrosynthesis-FGI, divergent vs. convergent syntheses. Synthesis of some typical organic molecules- Abscisic acid, Longifolene Ref. 1-9

2. Heterocyclic Chemistry (24 L)

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

b) Condensed five and six membered heterocycles:

Benzofuran, Indole, Quinoline

c) Condensed five membered heterocycles:

Benzoxazole, Benzthiazole, Benzimidazole

d) Synthesis of ranitidine, papavarine, amlodipine, bromouridine, tryptophan, thiamine, chloroquine Ref. 10-17

References:

1. Designing of organic synthesis –S.Warren (Wiley)
2. Some modern methods of organic synthesis–W.Carruthers (Cambridge)
3. Organic chemistry– J.Clayden, N.Greeves,S.Warren andP. Wothers (Oxford Press)
4. Organic synthesis –Michael B.Smith
5. Advanced organic chemistry, Part B–F.A Careyand R.J. Sundberg, 5th edition (2007)
6. Guide book to organic synthesis-RK Meckie, DM Smith and RA Atken
7. Organic synthesis-Robert E.Ireland
8. Strategic Applications of named reactions in organic synthesis-Laszlo Kurtiand Barbara Czako
9. Organic synthesis through disconnection approach-P.S.Kalsi
10. Heterocyclic Chemistry-T. Gilchrist
11. An introduction to the chemistry of heterocyclic compounds-R M.Acheso
12. Heterocyclic Chemistry-JA Jouleand K Mills
13. Principles of modern heterocyclic chemistry-A Paquette
14. The essence of Heterocyclic Chemistry- A.R. Parikh, Hansa Parikh, Ranjan Khunt
15. Handbook of Heterocyclic Chemistry-AR Katritzky, AF Pozharskii
16. Heterocyclic Chemistry-II- R. R.Gupta, MKumar, VGupta, Springer (India) pvt
17. Heterocyclic Chemistry-R. K.Bansal

Choice Based Credit System Syllabus
(2019 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III)

Subject: Organic Chemistry

Course: Designing of org. synthesis and Heterocyclic Chemistry **Course Code:** CHO-5301

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Program Outcomes (POs) and Course Outcomes (COs) Matrix with Weightage:

Course Outcomes	Programme Outcomes(POs)								
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	2
CO2	2	2	0	3	0	0	0	0	0
CO3	1	3	0	0	0	0	0	0	0
CO4	2	0	0	2	3	0	0	0	0
CO5	1	3	0	2	2	0	0	0	0
CO6	3	3	0	0	0	3	0	0	2
CO7	0	0	0	2	2	0	3	0	3

Justification for the mapping

PO1 (Disciplinary Knowledge):

- CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis.
- CO2. Expertise in reactions using protection and deprotection methods.
- CO3. Demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.
- CO4. Describe methods for synthesis and transformation of the most common functional groups
- CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
- CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

PO2 (Critical Thinking and Problem Solving):

- CO2. Expertise in reactions using protection and deprotection methods.
- CO3 demonstrate the skill of critical thinking for retrosynthesis of largest molecule and can able to synthesize them by designing simple organic methodology.
- CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
- CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis.

PO4 (Research-related Skills and Scientific Temper):

- CO2. Expertise in reactions using protection and deprotection methods.
- CO4. Describe methods for synthesis and transformation of the most common functional groups.
- CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach.
- CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO5 (Trans-disciplinary Knowledge):

CO4. Describe methods for synthesis and transformation of the most common functional groups.

CO5. Identify, analyse and evaluate synthetic routes to target molecules using retrosynthetic approach

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO6 (Personal and Professional Competence):

CO1 Get the knowledge of designing the new molecule and heterocyclic compound synthesis.

CO 6 Apply the knowledge of organometallic reagents and reactions in organic synthesis

PO7 (Effective Citizenship and Ethics):

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

PO9 (Self-directed and Life-long Learning):

CO1. Get the knowledge of designing the new molecule and heterocyclic compound synthesis

CO6. Apply the knowledge of organometallic reagents and reactions in organic synthesis

CO7. Get hold of the ability to engage in independent and life-long learning of Functional group interconversion and protective group methodology.

CHO-5302: Spectroscopic Methods in Structure Determination (48 L+ 12 T) (4 Credit)

Course Objective: On completion of the course, the student will be able to:

- 1) Students will gain knowledge about the instrumentation used in NMR, IR, and Mass Spectroscopy, including the components and operation of the instruments.
- 2) Students will assign peaks in NMR spectra, correlating NMR data with molecular structure, and using IR and Mass Spectroscopy data to support structural assignments.
- 3) Students will learn the fundamental principles and theory behind NMR, IR, and Mass Spectroscopy techniques.
- 4) Students will develop the skills to interpret NMR, IR, and Mass Spectroscopy spectra, including identifying functional groups, determining chemical shifts, analyzing peak patterns, and understanding fragmentation patterns in Mass Spectroscopy.
- 5) Students will also learn data analysis techniques, such as peak integration and spectral manipulation.
- 6) Students will explore the various applications of NMR, IR, and Mass Spectroscopy in chemistry, such as identifying unknown compounds, monitoring chemical reactions, and studying molecular dynamics.
- 7) Students will learn how to use NMR, IR, and Mass Spectroscopy data to determine the structure of organic compounds.

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Understand the principles and theory behind different spectroscopic methods.
- CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.
- CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.
- CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.
- CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.
- CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.
- CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis.

¹H NMR Spectroscopy**(14L)**

Recapitulation of basic principle, Fourier Transform technique, Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant “*J*”, classification of spin system like AB, AX, AX₂, ABX, AMX, ABC, A₂B₂. Spin decoupling, Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear over-hauser effect (NOE), and resonance of other nuclei like ³¹P

¹³C NMR spectroscopy**(8 L)**

FT NMR, Types of ¹³C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT with 3 different angles, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, chemical shifts of solvents, Homo nuclear (¹³C-¹³C) and Hetero nuclear (¹³C-¹H) coupling constants.

2D NMR Techniques**(6L)**

General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)-Homo COSY (¹H-¹H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications. Illustrative example of COSY, HSQC in carbohydrate characterization.

Mass Spectrometry**(10L)**

Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupole mass filter, time of flight (TOF)). Rules of fragmentation of different functional groups, factors controlling fragmentation

Problems based on joint application of UV, IR, PMR, CMR, and Mass.**(10 L)**

(Including reaction sequences)

References:

1. Introduction to Spectroscopy-D.L. Pavia, G.M. Lampman, G.S. Kriz,3rdEd. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wileyand Sons.
3. Spectroscopic methods in organic chemistry-D.H.WilliamsandI.FlemmingMc Graw Hill
4. Absorption spectroscopy of organic molecules - V. M. Parikh
5. Nuclear Magnetic Resonance-Basic Principles-Atta-Ur-Rehman, Springer-Verlag (1986).
6. One and Two dimensional NMR Spectroscopy-Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis-Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998)
8. Organic structural Spectroscopy-Joseph B.Lambert, Shurvell, Lightner,Cooks, Prentice-Hall (1998).
9. Organic structures from spectra -Field L.D., Kalman J.R. and Sternhell S.4th Ed. John Wiley and sons Ltd.
10. Spectroscopic identification of organic compound-R.M.Silverstein, G.C.Basslerand T.C.Morril, JohnWiley
11. Introduction to NMR spectroscopy-R.J.Abrahm, J.FisherandP.loftus Wiley
12. Organic spectroscopy-Williamkemp, E. L.B. with Mc Millan
13. Spectroscopy of organic molecule-P.S.Kalsi, Wiley,Esterna, New Delhi
14. Organic spectroscopy-R.T.Morrison and R.N.Boyd
15. Practical NMR spectroscopy-M.L. Martin, J.J. Delpenach, andD. J. Martyin
16. Spectroscopic methods inorganic chemistry-D.H. Willson,I.Fleming
17. Spectroscopy in organic chemistry-C. N.R. Rao andJ. R. Ferraro
18. NMR-Basic principle and application-H. Guntur
19. Interpretation of NMRs pectra-RoyH.Bible
20. Carbohydrate Characterization through Multidimensional NMR: An Undergraduate Organic Laboratory Experiment. *J. Chem. Educ.* **2020**, 97(1), 195-199
21. Mass spectrometry organic chemical applications-JH Banyon

Choice Based Credit System Syllabus
(2019 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III)

Subject: Organic Chemistry

Course: Spectroscopic Methods in Structure Determination

Course Code: CHO-5302

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	2	0	1	0	0	0
CO2	2	3	0	0	0	2	0	0	0
CO3	3	3	0	0	2	0	0	0	0
CO4	1	0	0	3	0	2	0	0	0
CO5	1	2	0	2	3	0	0	0	0
CO6	3	0	0	2	0	3	0	0	2
CO7	1	3	0	0	0	2	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Understand the principles and theory behind different spectroscopic methods.

CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.

CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.

CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.

CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO2 (Critical Thinking and Problem Solving)

CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.

CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.

CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO4 (Research-related Skills and Scientific Temper):

CO1. Understand the principles and theory behind different spectroscopic methods.

CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.

CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

PO5 (Trans-disciplinary Knowledge):

CO3. Analyze IR spectra to identify functional groups and determine the presence of specific bonds.

CO5. Apply UV-visible spectroscopy to determine the electronic transitions and conjugation in organic compounds.

PO6 (Personal and Professional Competence):

CO1. Understand the principles and theory behind different spectroscopic methods.

CO2. Interpret NMR spectra to determine the connectivity and functional groups present in organic compounds.

CO4. Utilize mass spectrometry to determine the molecular weight and fragmentation pattern of organic compounds.

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

CO7. Develop critical thinking and problem-solving skills in the context of spectroscopic analysis

PO9 (Self-directed and Life-long Learning):

CO6. Integrate multiple spectroscopic techniques to solve complex structural problems.

CHO-5303: Organic Stereochemistry-I and Organic Reaction Mechanism (48L+12T) (4Credit)

Course Objective: On completion of the course, the student will be able to:

- 1) To explore the reactivity patterns and synthetic methods involving carbanions, including their generation, stability, and reactions with electrophiles.
- 2) To understand the factors that influence carbanion stability and the use of carbanions in carbon-carbon bond formation.
- 3) To study the formation, reactivity, and synthetic applications of enamines, which are versatile intermediates in organic synthesis.
- 4) To study the stereochemistry of reactions involving six-membered and fused bridge cage ring compounds.
- 5) To explore the different conformations and their energy profiles of six-membered and fused bridge cage ring compounds. This includes understanding the factors that influence conformational stability and the interconversion between different conformers.
- 6) To gain a deep understanding of the stereochemistry of six-membered and fused bridge cage ring compounds, enabling them to analyze and predict stereochemical outcomes in reactions, design synthetic routes.
- 7) To study the formation, reactivity, and synthetic applications of enamines, which are versatile intermediates in organic synthesis.
- 8) To understand the principles and mechanisms of various types of neighboring group participation, such as anchimeric assistance and neighboring group assistance

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Understand the principles and concepts of stereochemistry, including stereoisomerism, chirality, enantiomers, diastereomers, and their importance in organic chemistry.
- CO2. Apply the principles of stereochemistry to predict the three-dimensional arrangement of molecules or functional groups in a given compound.
- CO3. Recognize the various factors that influence the stability and reactivity of stereoisomers, including steric hindrance, ring strain, and electronic effects.
- CO4. Students will be able to identify and describe the key steps and intermediates involved in organic reactions.
- CO5. Students will be able to predict the regiochemistry and stereochemistry of organic reactions based on a given reaction mechanism.
- CO6. Students will be able to propose a reasonable mechanism for a given reaction, including the use of curly arrows to indicate electron movement

CO7. Students will be able to apply the principles of organic reaction mechanisms to design efficient and selective synthetic routes for the synthesis of organic compounds.

Organic Stereochemistry-I

1. Stereochemistry of six membered rings. Ref.1,3, 4,5 (11 L)
2. Stereochemistry of rings other than six membered Ref.1, 3, 4,5 (7 L)
3. Fused Bridged and caged rings Ref.1,2,3, 4 (6 L)

Organic Reaction Mechanism

1. Carbanions: Formation, geometry, stability and related reactions- Aldol, α -halogenation, haloform reaction, Michael reaction, Robinson annulations, Mannich, Stobbe, Cannizaro's, Darzens, Dieckmann, Knoevenagel, Benzoin, Perkin, Benzoin condensation, Grignard, Claisen condensation, Baylis-Hilman, Appel reaction, Corey-Fuchs reaction Ref.6,7,8,10 [12 L]
2. Enamines: formation and applications of enamine in organic synthesis. Ref.9 [4 L]
3. NGP: Neighbouring group participation Ref. 6 [4 L]
4. Synthesis and reactions of carbenes and nitrenes Ref.9 [4 L]

References:

1. Stereochemistry of carbon compounds- E.L. Eliel
2. Stereochemistry of carbon compounds- E.L. Elieland S. H. Wilen
3. Stereochemistry of organic compounds–Nasipuri
4. Stereochemistry of organic compounds-Kalsi
5. Organic stereochemistry–Jagdamba Singh
6. Mechanism and structure in Organic Chemistry–E.S.Gould (Holt, Rinehartand Winston)
7. Advanced organic chemistryby J. March, 6th Ed.
8. Advanced organic chemistry.F.A. Careyand R.J.Sundberg, PartA 5thEd.Springer (2007)
9. Advanced organic chemistry. F.A. Carey and R.J.Sundberg, PartB5thEd. Springer(2007)
10. Organic Chemistry–J.Clayden,N. Greeves,S.WarrenandP. Wothers

Choice Based Credit System Syllabus
(2019 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III)

Subject: Organic Chemistry

Course: Org. Stereochemistry-I and Org. Reaction Mechanism **Course Code:** CHO-5303

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	2	0	2	0	0	0
CO3	1	0	0	0	3	0	0	0	0
CO4	3	3	0	2	0	2	0	0	0
CO5	3	0	0	0	3	3	0	0	0
CO6	2	3	0	0	0	3	0	0	2
CO7	1	3	0	2	0	2	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Understand the principles of stereochemistry and apply them to analyze the stereochemistry of six-membered rings, rings other than six-membered, fused bridged, and caged rings.

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions

CO3. Explain the formation and applications of enamines in organic synthesis.

CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.

CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.

CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO2 (Critical Thinking and Problem Solving):

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions.

CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.

CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO4 (Research-related Skills and Scientific Temper):

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions

CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.

CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO5 (Trans-disciplinary Knowledge):

CO3. Explain the formation and applications of enamines in organic synthesis.

CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.

PO6 (Personal and Professional Competence):

CO1. Understand the principles of stereochemistry and apply them to analyze the stereochemistry of six-membered rings, rings other than six-membered, fused bridged, and caged rings.

CO2. Demonstrate knowledge of organic reaction mechanisms, including the formation, geometry, and stability of carbanions, and apply this knowledge to related reactions

CO4. Understand and describe the concept of neighboring group participation (NGP) in organic reactions.

CO5. Discuss the synthesis and reactions of carbenes and nitrenes in organic chemistry.

CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

CO7. Develop research-related skills and scientific temper by critically evaluating and analyzing organic stereochemistry and reaction mechanism literature.

PO9 (Self-directed and Life-long Learning):

CO6. Apply critical thinking and problem-solving skills to analyze and solve complex organic stereochemistry and reaction mechanism problems.

CHO-5304:Photochemistry, Free radicals and Pericyclic Reactions and (48L+12T)(4Credit)

Course Objective: On completion of the course, the student will be able to:

- 1) Students will learn to analyze and interpret the mechanisms of pericyclic reactions using molecular orbital theory
- 2) Students will explore the synthetic applications of pericyclic reactions, including their use in the construction of complex organic molecules and the synthesis of natural products.
- 3) To provide students with a comprehensive understanding of the fundamental principles underlying photochemical reactions in organic chemistry.
- 4) Students will develop a solid understanding of the theoretical principles and concepts that govern pericyclic reactions, including orbital symmetry, frontier molecular orbital theory, and the Woodward-Hoffmann rules.
- 5) Students will learn to recognize and differentiate between various types of pericyclic reactions, such as cycloadditions, electrocyclic reactions, sigmatropic rearrangements.
- 6) Students will explore the synthetic applications of pericyclic reactions, including their use in the construction of complex organic molecules and the synthesis of natural products.
- 7) Students will learn about the nature, properties, and reactivity of free radicals in organic chemistry.

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Students will learn the fundamental concepts of photochemistry, including the interaction of light with organic molecules, absorption and emission of photons, and the role of excited states in chemical reactions.
- CO2. Students will gain an understanding of various photochemical reactions, such as photoisomerization, photodimerization, photorearrangement, and photodegradation. They will learn about the mechanisms and factors that influence these reactions.
- CO3. Students will explore the use of photochemical reactions in organic synthesis, including the synthesis of complex molecules and the development of new synthetic methodologies. They will learn about the advantages and limitations of photochemical transformations
- CO4. Students will gain a thorough understanding of free radicals, their structure, stability, and reactivity in organic compounds.
- CO5. Students will learn about various radical reactions, including radical addition, radical
- CO6. Substitution, and radical rearrangement, and their mechanisms.
- CO7. Students will explore the use of radical reactions in the synthesis of complex organic compounds, such as the synthesis of natural products, pharmaceuticals, and polymers.

CO8. Students will learn the fundamental concepts and theories behind pericyclic reactions, including the Woodward-Hoffmann rules and the conservation of orbital symmetry.

1. Photochemistry

(16 L)

General basic principles, photochemistry of carbonyl compounds, alkenes, dienes and aromatic compounds and their application in organic synthesis (Norrish type I and II reaction, isomerization, Paterno-Buchi reaction) photo rearrangements (di- π -methane, oxa di- π and aza di- π -methane rearrangements), photoreduction, photosubstitution reaction-Barton reaction.

Photochemistry in nature- chemistry of vision, Application of photochemical reactions in synthesis– Isocomene Ref. 1,2,3,4

2. Free radicals:

[16 L]

Generation of radicals, Stability of Free Radical, types of free radicals, Nucleophilic and electrophilic radicals, methods for detection and formation of free radicals, radical initiators, Characteristics reactions,-Free radical substitution, addition to multiple bonds, free radical halogenation-chlorination and bromination-NBS, autoxidation, Thermal decomposition of hydroperoxides, Radicals in synthesis: Hunsdiecker reaction, Barton Nitrite Photolysis reaction, Barton Decarboxylation, Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors, cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling. C-C bond formation in aromatics, S_NAr reactions-Sandmeyer reaction Ref. 1, 3, 6

3. Pericyclic reactions

[16 L]

Recapitulation of Molecular Orbitals, their symmetry properties, Woodward –Hoffmann's Conservation of orbital symmetry property rule. Application of Woodward –Hoffmann's Conservation of orbital symmetry property rule to the ground state and excited state Electrocyclic reactions, Cycloaddition reactions, Chelotropic reactions, Sigmatropic reactions, and 1,3-dipolar additions, Analysis by correlation diagrams, FMO approach, Mobius-Huckel theory and ATS concept. Application of pericyclic reactions: Ene reaction, Sommelet-Hauser rearrangement, Claisen and Cope rearrangements, fluxional molecules, synthesis of Endiandric acid. Ref. 1, 3, 5, 7, 10-14

References:

1. Advanced Organic Chemistry, Part A – F.A. Carey and R.J. Sundberg, 5th Ed. Springer (2007)
2. Excited states in Organic Chemistry – J.A. Barltrop and J.D. Coyle, John Wiley & Sons

3. Photochemistry and Pericyclic reactions-Jagdamba Singh,Jaya Singh 3rdEd.
4. Organic photochemistry: A visual approach-Jan Kopecky, VCH publishers (1992).
5. Conservation of orbital symmetry–R.B.Woodward and R.Hoffmann;Verlag Chemie, Academic press (1971).
6. Radicals in Organic SynthesisB. Giese, Pergamonpress (1986)
7. Orbital Symmetry:A problem solving approach-R.E.LehrandA.P. Marchand; Academic (1972)
8. Classics in total synthesis-K.C. Nicolaou and E.J.Sorensen;VHC (1996)
9. P.A. Wenderand J. J. Howbert *J. Am. Chem. Soc.* **1981**,103, 688-690.
10. Organic reactions and orbital symmetry, 2ndEd.T.L.Gilchrist andR.C.Storr
11. Organic Chemistry–J.Clayden,N. Greeves,S.WarrenandP. Wothers
12. Pericyclic reactions:A textbook–S.Sankararaman
13. Pericyclic reactions-GillandWillis
14. Frontier orbitals and organic chemical reactions-IanFleming, John Wiley & sons

Choice Based Credit System Syllabus
(2019 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III)

Subject: Organic Chemistry

Course: Photochemistry, Free radicals and Pericyclic Reactions **Course Code:** CHO-5304

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	0	0	3	0	0	0
CO3	0	3	0	2	0	0	0	0	0
CO4	3	3	0	0	0	3	0	0	0
CO5	3	0	0	2	0	2	0	0	0
CO6	3	3	0	0	2	3	0	0	2
CO7	0	0	0	2	2	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Understand the principles and mechanisms of photochemical reactions, including photo rearrangements, photo reduction, and photo oxidation.

CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.

CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.

CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and Barton Nitrite Photolysis reaction.

CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

PO2 (Critical Thinking and Problem Solving):

CO2, CO3, CO4, and CO6 exhibit a strong alignment, indicating a focus on developing critical thinking skills in the context of photochemical reactions and their applications.

CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.

CO3. Utilize photochemical reactions in synthesis, specifically the Isocomene synthesis.

CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.

CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

PO4 (Research-related Skills and Scientific Temper):

CO3, CO5, and CO7 show a moderate alignment, indicating a focus on research-related skills, especially in utilizing photochemical reactions in synthesis and explaining the chemistry of vision.

- CO3. Utilize photochemical reactions in synthesis, specifically the Isocomene synthesis.
- CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and Barton Nitrite Photolysis reaction.
- CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO5 (Trans-disciplinary Knowledge):

- CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.
- CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO6 (Personal and Professional Competence):

- CO1. Understand the principles and mechanisms of photochemical reactions, including photo rearrangements, photo reduction, and photo oxidation.
- CO2. Apply the concepts of photochemistry to analyze and predict the outcomes of photo substitution reactions, such as the Barton reaction.
- CO4. Describe the characteristics and reactions of free radicals, including free radical substitution and addition to multiple bonds.
- CO5. Apply free radicals in various synthetic reactions, such as the Hunsdiecker reaction and Barton Nitrite Photolysis reaction.
- CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.
- CO7. Explain the chemistry of vision and the role of photochemical reactions in natural processes.

PO9 (Self-directed and Life-long Learning):

- CO6. Understand the principles and applications of pericyclic reactions, including cycloaddition reactions, chelotropic reactions, and 1,3-dipolar additions.

Practical course I

CHO-5305: Single stage preparations [4Credits]

Course Objective: On completion of the course, the student will be able to:

- 1) Develop practical skills in handling and manipulating organic compounds, including proper techniques for weighing, measuring, and transferring reagents, as well as safe handling and disposal of hazardous materials
- 2) Develop practical skills in handling and synthesizing organic compounds
- 3) Develop an understanding of the fundamental principles and concepts of the isolation of natural products, including extraction techniques, purification methods
- 4) Gain knowledge about the principles and mechanisms of reduction reactions
- 5) Understand the principles and mechanisms of formylation reactions and gain practical experience through formylation experiments,
- 6) Acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds, such as cyclization reactions, functional group transformations,
- 7) Develop proficiency in performing organic synthesis and purification techniques, including the use of appropriate laboratory equipment and methods for the synthesis and purification

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
- CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
- CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.

CO7. Developing practical skills in handling and manipulating organic compounds.

At least nine single stage and five isolation of Natural products and two quantitative analysis should be carried out. The preparation should be carried out on micro scale.

A) Advanced organic practical (any 9)

- a) Preparation of dry solvent seg THF, DCM, DMF, DMSO, CH₃CN
- b) Synthesis and purification and characterization
 - 1) Ethyl cinnamate from benzaldehyde (Wittig reaction)
 - 2) 2-phenylindole by Fischer indole synthesis
 - 3) Cyclohexanone to enamine
 - 4) Triphenylmethyl diphenyl methyl carbinol (Grignard reaction)
 - 5) 4-chlorotoluene from p-toluidine (Sandmeyer reaction)
 - 6) Cyclohexanol from cyclohexanone (NaBH₄ reduction)
 - 7) Glucose pentaacetate from glucose
 - 8) Stilbene from benzyl chloride (Wittig reaction)
 - 9) Vilsmeier-Haack formylation of 2-methoxynaphthalene
 - 10) Diels-Alder reaction of anthracene and maleic acid.
 - 11) 4-Nitrobenzotrile from 4-nitrobenzaldehyde
 - 12) Quinoline from Aniline (Skraup synthesis)
 - 13) Synthesis of imidazo[1,2-a]pyridines
 - 14) 1-phenyl,3-methylpyrazole-5-one from phenylhydrazine and ethyl acetoacetate

B) Isolation of Natural products (Any 5)

- 1) Caffeine from tea leaves (Soxhlet extraction)
- 2) Piperine from pepper (Soxhlet extraction)
- 3) Lycopene from tomatoes
- 4) Trimyristin from nutmeg
- 5) Eugenol from clove
- 6) Curcumin from turmeric powder
- 7) Casein and lactose from milk
- 8) β -Carotene from carrots

C) Organic quantitative analysis (any 2)

- 1) Estimate amount of sulphadiazine present in given tablet
- 2) Estimation of paracetamol and ibuprofen in given tablet
- 3) Estimation of glucose using Fehling's solution
- 4) Estimation of sucrose using Fehling's solution
- 5) Estimation of amino acid by formol titration

Choice Based Credit System Syllabus
(2019 Pattern)

**Mapping of Program Outcomes with Course
Outcomes**

Class: M.Sc. II (SEM III)
Chemistry

Subject: Organic

Course: Single stage preparations

Course Code: CHO-5305

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	2	0	3	0	0	2
CO2	3	3	0	2	2	3	0	0	2
CO3	3	3	0	2	0	0	0	0	0
CO4	3	3	0	3	2	0	0	0	2
CO5	3	3	0	0	0	3	0	0	2
CO6	0	3	0	2	2	3	0	0	2
CO7	3	0	0	0	0	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

- CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
- CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
- CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
- CO7. Developing practical skills in handling and manipulating organic compounds.

PO2 (Critical Thinking and Problem Solving):

- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
- CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
- CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO4 (Research-related Skills and Scientific Temper):

- CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO3. Students will gain knowledge about the principles and mechanisms of reduction reactions and performing reduction reactions using various reducing agents, such as metal hydrides.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO5 (Trans-disciplinary Knowledge):

- CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.

PO6 (Personal and Professional Competence):

- CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.
- CO7. Developing practical skills in handling and manipulating organic compounds.

PO9 (Self-directed and Life-long Learning):

- CO1. Students will gain proficiency in performing organic synthesis and purification techniques.
- CO2. Students will acquire hands-on experience in performing various synthetic methods and techniques specific to the synthesis of heterocyclic compounds.
- CO4. Through formylation experiments, students will understand principles and mechanisms of formylation reactions.
- CO5. Enhancing communication skills by effectively documenting experimental procedures and results.
- CO6. Understanding the fundamental principles and concepts of isolation of natural products.

Practical course II

CHO-5306: Double and multiple stage preparations 4 credits]

Course Objective: On completion of the course, the student will be able to:

- 1) To develop students' skills in designing multi-step synthetic routes based on the selection of appropriate reactions and reagents.
- 2) To introduce students to practical laboratory techniques commonly used in multi-step organic synthesis, including purification methods, separation techniques, and characterization techniques (such as spectroscopy).
- 3) To enhance students' problem-solving skills and critical thinking abilities by providing them with opportunities to analyze complex synthetic problems and propose efficient solutions.
- 4) To emphasize reagents or reactions.
- 5) To teach students to break down complex target molecules into simpler, readily available starting materials using retrosynthetic principles. This involves identifying key functional groups and strategic disconnections.
- 6) To familiarize students with a wide range of reactions and techniques for the conversion of one functional group into another.
- 7) Understanding reaction mechanisms, regioselectivity, and stereoselectivity.
- 8) the importance of safety protocols and ethical considerations in the practice of organic chemistry, particularly in multi-step synthesis involving potentially hazardous

Course Outcomes : On completion of the course, the student should be able to:

- CO1. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.
- CO2. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.
- CO3. Developing critical thinking skills to evaluate the advantages and limitations of different
- CO4. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.
- CO5. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.
- CO6. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.
- CO7. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.

At least five double stage and two multiple stage preparations should be carried out. The preparation should be carried out on micro scale.

A) Double stage preparation(any5)

- 1) Benzaldehyde to benzalacetophenone to epoxide
- 2) Phthalimide to *N*-benzylphthalimide to benzylamine
- 3) Cyclohexanone to phenylhydrazone to 1,2,3,4-tetrahydrocarbazole
- 4) Hydroquinone to hydroquinonediacetate to 2,5-dihydroxyacetophenone
- 5) Resorcinol to 4-methyl-7-hydroxycoumarin to 4-methyl-7-acetoxycoumarin
- 6) Phthalic acid to phthalimide to anthranilic acid
- 7) Hydroquinone to hydroquinone diacetate to 1,2,4-triacetoxybenzene
- 8) Synthesis of indigo and its vat dyeing of cotton
- 9) Acetanilide to 4-nitroacetanilide to 4-nitroaniline

B) Multiple stage preparations(any2)

- 1) Glycine to Hippuric acid to Azalactone to 4-Benzylidene-2-phenyl oxazol-5-one
- 2) Aldehyde to benzoin to benzil to benzilic acid
- 3) Acetanilide to *p*-acetamido benzene sulphonyl chloride to *p*-acetamido benzene sulphonamide to sulphanilamide.
- 4) D-glucose to 1,2,5,6-Di-*O*-isopropylidene- α -D-glucofuranose to S-methyl dithiocarbonate derivative to 3-deoxy-1,2,5,6-Di-*O*-isopropylidene- α -D-glucofuranose

Choice Based Credit System Syllabus
(2019 Pattern)

Mapping of Program Outcomes with Course Outcomes

Class: M.Sc. II (SEM III)

Subject: Organic Chemistry

Course: Double and multiple stage preparations

Course Code: CHO-5306

Weightage: 1=weak or low relation, 2= moderate or partial relation, 3=strong or direct relation

Course Outcomes (COs) and Program Outcomes (POs) Matrix with Weightage:

CO/PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CO1	3	0	0	0	0	3	0	0	0
CO2	3	3	0	0	0	3	0	0	0
CO3	3	3	0	2	0	0	0	0	0
CO4	3	0	0	0	2	0	0	0	0
CO5	3	0	0	3	0	3	0	0	0
CO6	3	3	0	2	0	3	0	0	1
CO7	0	3	0	2	2	3	0	0	0

Justification for the mapping

PO1 (Disciplinary Knowledge):

CO1. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.

CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.

CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.

CO4. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.

CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.

PO2 (Critical Thinking and Problem Solving):

CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.

CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.

CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.

CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO4 (Research-related Skills and Scientific Temper):

CO3. Developing skills in designing and planning synthetic routes for the preparation of heterocyclic compounds using the mentioned reactions.

CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.

CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.

CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO5 (Trans-disciplinary Knowledge):

CO4. Gaining proficiency in performing laboratory techniques and procedures involved in the double stage preparation.

CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO6 (Personal and Professional Competence):

CO1. Understanding the principles and mechanisms of nitration, sulphonation, oxidation, reduction, and hydrolysis reactions in double stage preparation.

CO2. Acquiring knowledge of the various reagents, catalysts, and conditions used in these reactions for the synthesis.

CO5. Analyzing and interpreting experimental data obtained from the reactions to assess the success and purity of the synthesized compounds.

CO6. Enhancing problem-solving abilities by troubleshooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.

CO7. Developing critical thinking skills to evaluate the advantages and limitations of different synthetic approaches for the preparation of organic compounds.

PO9 (Self-directed and Life-long Learning):

CO6. Enhancing problem-solving abilities by trouble shooting and optimizing reaction conditions to improve the yield and selectivity of the desired compounds.