Name of the Programme: M. Sc -I (Organic Chemistry)

Course Code: CHO-502 **Title of the course:** Pericyclic and Organic Photochemical Reactions

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied organic chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. To introduce various concepts in pericyclic chemistry based on molecular orbital theory and apply for solving pericyclic reactions 2. To introduce analysis of pericyclic reactions using theoretical concepts. 3. To learn mechanistic aspects of pericyclic & photochemical reactions in organic synthesis.	
Content	**1. Pericyclic Reactions** a. Theory of pericyclic reactions i. Frontier Molecular Orbital (FMO) theory ii. Transition state aromaticity (Mobius-Huckel theory) concept iii. Orbital correlation diagram method. b. Analysis of pericyclic reactions (including stereochemistry) using the above concepts i. Cycloaddition reactions ii. Electrocyclic reactions iii.Sigmatropic rearrangements under thermal and photochemical conditions (Note: Various important features to be discussed taking examples important reactions of each type) c. Some synthetically useful reactions (examples via theory of pericyclic reaction). d. Diels–Alder and retro Diels-Alder reaction: Regiochemistry, stereochemistry and intramolecular reactions. e. 1, 3-dipolar additions f. [3, 3]-Shifts; Claisen and Cope, aza-Cope-, oxy-Cope rearrangements and fluxional molecules, variants of Claisen Rearrangement such as Johnson-Claisen, Eschenmoser-Claisen, Carroll- Claisen and Ireland-Claisen. g. [2,3]-Sigmatropic rearrangements such as Sommelet-Hauser rearrangement, Sulfonium ylide rearrangement, Meisenheimer rearrangement, Wittig rearrangement, Mislow-Evans rearrangement h. Ene reaction, hetero-ene, retro-ene reactions i. [1,5]-Thermal and [1,7]-photochemical sigmatropic hydrogen shifts	No of hours 34
	2. Organic Photochemistry	26

	a. Interaction of electromagnetic radiation with matter, laws of photochemistry; fateof excited molecule; principles of energy transfer, types of photochemical reactions. Theoretical concepts in organic photochemistry w. r. t. cycloadditions, Electrocyclicreactions and sigmatropic reactions b. Photochemical reactions of alkenes, dienes, carbonyl compounds and arenes including the following- geometrical isomerisation: *Cis-trans* isomerization andphotostationary equilibrium; Paterno-Buchi reaction; Norrish Type cleavages; Di-pimethane rearrangement; bicycle rearrangement c. Photochemistry of aromatic compounds: valance isomerization; photostationary state of benzene and azabenzenes. [4+4]-photodimerization of derivatives of naphthalenes. cycloaddition reaction of benzene, naphthalene, pyrrole and indoles with alkenes and alkynes d. Reactions involving singlet and triplet oxygen: Photooxygenation reactions, examples of [2+2] and [4+2]-cycloaddition reaction with isocyclic, heterocyclic, dienes and polynuclear aromatic compounds e. Applications of Organic Photochemistry: Photochemical Reactions as Key Steps in Natural Product Synthesis (any four examples); example of photopolymerization; photochemical functionalization at unactivated carbon: Barton reaction, the hypohalite reaction and the Hofmann-Loffler-Freytag reaction	
Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References / Readings	1. N. Turro, V. Ramamurthy, J.C. Scaiano, Modern Molecular Photochemistry of Organic molecules , University Science Books, 2010. 2. B. Dinda, Essentials of Pericyclic and Photochemical Reactions, Springer, 1st Ed. 2017. 3. S.Kumar, V. Kumar, S.P. Singh, Pericyclic Reactions: A Mechanistic and Problem-Solving Approach, Elsevier, 2016. 4. R. E. Lehr., A. P. Marchand, Orbital Symmetry: A Problem Solving Approach, Academic Press, 1972. 5. R. B. Woodward, R. Hoffmann, Conservation of Orbital Symmetry, Verlag chemie, Academic Press, NY, 1972. 6. I. Fleming, Frontier Orbitals and Organic Chemical Reactions, John Wiley & Sons, 1st Ed., 1991 7. T. L. Gilchrist, R. C. Storr, Pericyclic Reactions, Cambridge Univ. Press, 1972. 8. F. A. Carrey, R. J. Sundberg , Advanced Organic Chemistry Part A and B, Pelnum Pub., 3rd Ed. 1990. 9. T. Lowery, K. Richardson, Mechanisms and Theory in Organic Chemistry, Harper and Row Pub., NY, 3rd Ed., 1987.	

	10. C. H. DePay, Molecular Reactions and Photochemistry, Prentice Hall (I) Ltd, NewDelhi. 11. J. Kopecky, Organic Photochemistry- A Visual Approach, VCH Pub., 1992.
Course outcomes:	1. Students will be in a position to predict course of a given pericyclic reaction using the theoretical concepts. 2. Students will be able to apply knowledge of stereochemical output in a reaction. 3. Students will be able to understand and propose plausible mechanism of pericyclic/photochemical reactions. 4. Students will understand applications of organic photochemistry.