Course Code	Course Name	Credits
26CH509	PHOTOCHEMISTRY, PERICYCLICS AND REARRANGEMENTS	04

Course Objectives

- To understand the principles and mechanisms of organic photochemical and pericyclic reactions.
- To explain molecular rearrangements and important name reactions in organic synthesis.
- To develop the ability to analyze reaction pathways and predict outcomes based on orbital symmetry and reaction mechanisms.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand the principles and mechanisms of organic photochemistry including excited state behavior and photoreactions.
- Apply concepts of pericyclic reactions using molecular orbital symmetry, FMO theory, and correlation diagrams.
- Analyze molecular rearrangements and sigmatropic shifts in organic reaction mechanisms.
- Evaluate important name reactions and their applications in organic synthesis and reaction design.

Unit 1 - Organic Photochemistry (12 Hrs.)

Introduction; Franck–Condon principle; Jablonski diagram; characteristics of photochemical reactions; photoreduction, photooxidation, and photosensitization; photoreactions—Norrish Type I and II reactions; Paternò–Büchi reaction; photo-Fries rearrangement; photochemistry of alkenes, dienes, and aromatic compounds; di-π-methane rearrangement; reactions of unactivated centres; photochemistry of α,β-unsaturated carbonyl compounds; photochemical cycloadditions and rearrangements; photoadditions; Barton reaction.

Unit 2 – Pericyclic reactions I (12 Hrs.)

Molecular orbital symmetry; frontier molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, and allyl systems; classification of pericyclic reactions; FMO (Frontier Molecular Orbital) approach; Woodward–Hoffmann correlation diagram method and Perturbation Molecular Orbital (PMO) approach for explaining pericyclic reactions under thermal and photochemical conditions; electrocyclic reactions—conrotatory and disrotatory motions [(4n) and (4n + 2) systems]; allylic systems and secondary orbital effects.

Unit 3 - Pericyclic reactions II (12 Hrs.)

Cycloadditions—suprafacial and antarafacial additions; notation of cycloadditions; (4n) and (4n + 2) systems with emphasis on (2+2) and (4+4) cycloadditions; (2+2) cycloaddition of ketones; cheletropic reactions; secondary effects of substituents on the rates of cycloadditions; sigmatropic rearrangements—FMO and Perturbation Molecular Orbital (PMO) approaches for explanation under thermal and photochemical conditions; suprafacial and antarafacial shifts of hydrogen; sigmatropic shifts involving carbon moieties; retention and inversion of configuration; (3,3) and (5,5) sigmatropic rearrangements; Claisen and Cope rearrangements; fluxional tautomerism; aza-Cope rearrangements.

Unit 4 – Molecular Rearrangements (12 Hrs.)

Classification – electrophilic, nucleophilic and free radical rearrangements, mechanisms of the following rearrangements - pinacol–pinacolone, Wagner – Meerwin, Tiffenev-Demjanov, Dienone- Phenol, Favorskii, Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Stevens, Benzil – Benzilic acid, Brook and Benzidine, sommelet hauser rearrangement, rearrangements.

Unit 5 - Selected name reactions in organic synthesis (12 Hrs.)

Bayer-Villiger oxidation, Dakin reaction, Baker-Venkataraman reaction, Reformatsky reaction, Robinson annulation, Cannizzaro reaction, Dieckmann reaction, Perkin Reaction, Stobbe condensation, Bischler Napieralski reaction, Wittig rearrangement.

Reference Books:

1. R. T. Morrison, R. N. Boyd, and S. K. Bhattacharjee, Organic Chemistry, 7th Edn., 2011, Pearson Prentice Hall.
2. S. H. Pine, Organic Chemistry, Tata McGraw Hill, 5th Edn., 2008.
3. B. Michael Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 2007, John Wiley & Sons, 6th Edn.,
4. I. L. Finar, Organic Chemistry, Vol. 1 & 2, 5th Edn., 1975, Longman Ltd., New Delhi.
5. Peter Sykes, Guidebook to Mechanism in Organic Chemistry, 6th Edn., 1985, Longman Scientific & Technical,
6. S.M. Mukherjee, and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edn., 1990, Macmillan India Ltd., New Delhi.

Websites and eLearning Sources:

1. https://nptel.ac.in/courses/104106077https://www.youtube.com/watch?v=68qMmO0F6uU
2. https://nptel.ac.in/courses/104105462

COs and Bloom's Taxonomy Mapping – 26CH509		
Course Outcomes	**On completing P.G. program the students will be able to**	**BTL**
CO1	Understanding and recall of fundamental concepts in photochemistry, pericyclic reactions and rearrangements.	K1, K2
CO2	Apply the different methods and principles of photochemistry, pericyclic and rearrangement reactions to solve complex chemical problems and demonstrating synthesis.	K3
CO3	Analyzing complex chemical phenomena in photochemistry, pericyclic reactions, and rearrangements using a variety of experimental and theoretical methods.	K4
CO4	Evaluate and predict different types of photochemical, pericyclic and molecular rearrangement reactions and mechanisms.	K5
CO5	Proficiently create innovative solutions and experimental designs in photochemistry, pericyclic and rearrangements.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH509												
Course Outcomes	**Programme Outcomes (POs)**						**Programme Specific Outcomes (PSOs)**					**Mean Score of Cos**
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	
CO1	3	3	2	1	1	2	3	2	2	2	2	2.1
CO2	3	3	3	1	1	1	3	3	2	3	2	2.3
CO3	2	3	3	2	1	2	3	3	2	2	2	2.3
CO4	3	2	3	1	1	1	3	2	2	3	2	2.0
CO5	3	2	3	1	1	3	3	3	3	3	3	2.5
											Total	2.2

Mean Score: 3- High, 2- Medium/Moderate, 1-Low