Course Type	Course Code	Name of Course	L	Т	Р	Credit
DC	NCYC511	Physical Organic Chemistry	3	1	0	4

## **Course Objective**

- Fundamental aspects of reaction thermodynamics and kinetics and their applications in chemical transformations.
- Molecular orbital theory (MOT) and mechanism of organic reactions using MOT.
- Idea for visualizing molecules in three-dimensional projection.
- Introduction to the concept of chirality and chiral centers.
- Resolution of molecular complexity present in organic molecules through stereochemical analysis.

## **Learning Outcomes**

- Understanding of basic energetic and stereochemical requirements of a chemical reaction.
- Understanding of organic reaction mechanisms through Molecular Orbital Theory.
- Estimate the stability of various conformers of organic molecules by correlating steric, electronic and stereoelectronic effects.
- Prediction of the reaction outcome in a stereoselective reaction by establishing a preferred relative stereochemistry.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Title: Reaction Thermodynamics and Kinetics Types of mechanism, types, of reactions thermodynamic and kinetic requirements, kinetic and thermo- dynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, trapping of intermediates, methods of determining mechanisms, isotope effects. Elucidation of reaction mechanism-case studies.	7L + 2T	Understanding of organic reaction mechanisms using thermodynamic and kinetic parameters.
2	<b>Title: Molecular Orbital Theory</b> Basic description of bonding using molecular orbital theory, understanding of reaction mechanisms through molecular orbital theory bonding and structures of reactive intermediates (carbocations, carbanions, radicals and carbene); aromaticity, non- aromaticity and anti-aromaticity.	10L + 3T	Basic understanding of bonding and reactions of organic molecules using Molecular Orbital Theory.
3	Title: Conformation and reactivity of cyclic molecules Conformation analysis of cycloalkanes, cycloalkenes, decalines, hydrindanes, fused poly-cyclic systems, bridged ring systems. Effect of conformation on reactivity, methods of resolution, optical purity. Enantiotopic and diastereotopic atoms, groups & faces.	9L + 3T	Understanding of energetic and stereochemical requirements of organic reactions in cyclic molecules.

4	Title: Stereo-electronic effects in organic reactions Steric and Stereo-electronic effect in addition and ring-closure reactions: Baldwin's Rule and Dunitz's angle of attack, Cieplak Model. Zimmerman-Traxler transition state, Stereoselectivity and stereospecificity of 1,2- induction and 1,3-induction – Cram's rule and beyond, chelation-control and non-chelation- control, anomeric effect. Basics of stereospecific and stereoselective synthesis.	9L + 3T	Control of organic reactions using stereo-electronic effects. Determination of product selectivity under different reaction conditions.
5	Title: Stereochemistry and optical activity of organic molecules with heteroatom centers Stereochemistry of organo-nitrogen, organo- sulfur and organo-phosphorus compounds. Optical rotatory dispersion, circular dichroism, Cotton effect, axial haloketone rule, octant rule.	7L + 3T	Basic understanding of stereochemistry of organic molecules with nitrogen, sulfur and phosphorus center. Optical activity of organic molecules and their applications.
	Total	42L+14T	

## **Text Books:**

- 1. Modern Physical Organic Chemistry; Anslyn and Doherty, University Science Books, 2006.
- 2. Organic Chemistry: Jonathan Clayden, Nick Greeves and Stuart Warren. 2<sup>nd</sup> Edition, Oxford University Press, 2014
- 3. Stereochemistry of Organic Compounds, D. Nasipuri, 4th Edition, New Age International, 2020.
- 4. Stereochemistry of Organic Compounds, P.S. Kalsi, 11th Edition, New Age International, 2022.

## **Reference Books:**

- 1. Advanced Organic Chemistry, Jerry March, 7th Edition, John Wiley and Sons, 2015.
- 2. Stereochemistry of Organic Compounds, Elliel and Willen, 1st Edition, Wiley India, 2008.