

20CY103 ORGANIC CHEMISTRY - 1

Hours Per Week :

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4	-	-	4

COURSE DESCRIPTION AND OBJECTIVES:

This course offers students the thorough concept of bonding, chirality and thermodynamics for an organic reaction. VB theory, MO theory and Huckel's rule and electronic effects will be covered under the broad spectrum of bonding. Concepts of configuration, conformations and resolution of racemic compounds will be taught under stereochemistry. Finally, the thermodynamics and kinetics of reaction intermediates generated during the course of the reaction will help us to understand the enthalpy and entropy associated with the reaction.

COURSE OUTCOMES:

Upon completion of the course, the student will be able to achieve the following outcomes:

COs	Course Outcomes
1.	Construct the MO of organic molecules and understand their electronic criterion, substituent effect and field effect.
2.	Apply the concepts of chirality and optically active compounds to explain the importance of stereochemistry.
3.	Apply the concepts of conformational analysis and optical activity for resolution of some of the important acids, base and alcohols.
4.	Analyze the reactivity of different reaction intermediates in organic reactions.
5.	Apply the knowledge of thermodynamics and examine the reaction kinetics, and isotopic effects for an organic reaction.

UNIT-I

Bonding, MO theory, Aromaticity: M.O. and V.B. methods (Huckel's MO Method, pictorial representation of MOs for molecules, qualitative application of MO theory to reactivity). Inductive, resonance, hyper-conjugation and field effects, hydrogen bonding, Aromaticity and Huckel's rule (energy, structural, electronic criteria for aromaticity and relationship among them, aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticity). Concept of acids and bases: Effect of structure, substituent and solvent on acidity and basicity

UNIT - II

Stereochemistry: Configuration: stereogenic unit i) stereocenters: systems involving 1, 2, 3 centers, (D/L and R/S) descriptor, threo/ erythro / meso and syn/anti nomenclature. Representation of molecules in saw-horse, Fischer, and Newman formulae, symmetry element and molecular chirality. Stereo axis: chiral axis in allenes, spiro & biphenyls.

UNIT - III

Conformational Analysis and resolution: Cyclic stereochemistry: Baeyer strain theory, conformational analysis: cyclohexane, mono and disubstituted cyclohexane, symmetry properties, and optical activity. Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds, resolution of acids, bases and alcohols via diastereomeric salt formation.

UNIT - IV

Reactive Intermediates: Methods of formation, structure determination and reactions of the following reactive intermediates: carbocations, non-classical carbocations, carbanions, free radicals, carbenes and nitrenes, arynes and related species – Preliminary treatment.

UNIT - V

Thermodynamics and Kinetics: Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factors, intermolecular and intramolecular reaction. Heat of hydrogenation and heat of combustion. Application of thermodynamic principle in tautomeric equilibria [keto-enol tautomerism], Reaction kinetics; transition state theory, rate constant and free energy of activation, free energy profile for one step and two step reactions, catalytic reactions, kinetically controlled and thermodynamically controlled reactions, isotope effect, primary kinetic isotopic effect (K_H/K_D), principle of microscopic reversibility. Crossover experiments, Hammonds postulate, Curtin-Hammett Principle.

Text books:

1. Ian Fleming, Molecular Orbitals and Organic Chemical Reactions-Student Edition, Wiley, London, 2009.
2. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th edition, Pearson Education.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2nd Edition, 2012.

Reference Books

1. M. B. Smith and J. March, March Advanced Organic Chemistry, 6th edition, Wiley, 2007.
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Structure and Mechanisms, Part A, 5th Edition, Springer, 2007.