

Approval: 8th Senate Meeting

Course Name: Organic Reactions & Mechanism

Course Number: CY501

Credits: 3-1-0-4

Prerequisites: B.Sc. (with Chemistry) or Teachers consent

Intended for: UG/PG

Distribution: Core

Semester: Odd/Even

Course Preamble: The main objective of this course is to teach organic reaction mechanism that include nucleophilic, electrophilic, elimination and free radical reactions. Also, this course will provide an understanding on the relative stability of reactive intermediates which include carbocations, carbanions and free radicals. In addition, the students will be introduced with the mechanistic aspects of organic reactions to understand the relationship between structure and reactivity of organic compounds.

Course Outline:

Unit 1: Nucleophilic Substitution Reaction [14 Lectures]

Aliphatic Nucleophilic Substitution Reaction: The S_N2 , S_N1 , borderline of S_N1 and S_N2 mechanisms involving ion pairs and single electron transfer (SET) mechanisms. Relationship between stereochemistry and reaction mechanism. Neighbouring Group Participation, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. The S_{Ni} mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium.

Aromatic Nucleophile Substitution: The S_{NAr} , S_{N1} , benzyne and $S_{RN}1$ mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile.

Unit 2 : Electrophilic Substitution Reaction [10 Lectures]

Aliphatic electrophilic substitution reaction: S_{E1} , S_{E2} and S_{Ei} . The S_{E1} mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic electrophilic substitution reaction: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles.

Unit 3 : Elimination Reactions [5 Lectures]

The E₂, E₁ and E_{1c_B} mechanisms and their spectrum. Regiochemistry of elimination reactions and stereochemistry of E₂ elimination reactions. Reactivity; effects of substrate structures, attacking base, the leaving group and the medium. Concerted pyrolytic eliminations.

Unit 4 : Free Radical Reactions [6 Lectures]

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Addition to Carbon-Carbon Multiple Bonds: Free radical mediated cyclization reactions Baldwin rules.

Unit 5: Mechanistic and stereochemical aspects of other reactions [7 Lectures]

Addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration. Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds.

Text Books:

1. *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, F. A. Carey and R. A. Sundberg, , Fifth edition, Springer, New York, 2007
2. *Advanced Organic Chemistry – Reaction mechanism*) by Reinhard Bruckner, Academic Press, 2002.
3. *Organic Chemistry* by Jonathan Clayden, Nick Greeves, Stuart Warren, Oxford University Press, 2001
4. *Advanced Organic Chemistry* by J. March, John Wiley & Sons, 1992
5. *Organic Chemistry* by S. H. Pine, McGraw Hill, 1987.

Reference:

1. *Modern Synthetic Reactions* by H. O. House, W.A. Benjamin, Inc., 1972
2. *Understanding Organic Reaction Mechanism* by A. Jacobs, Cambridge 1998.
3. *Organic Chemistry* by J. M. Hornback, Books Coley, 1998.
4. *Organic Chemistry* by P.Y. Bruice, Prentice Hall, 1998.
5. *Organic Reaction and their Mechanism* by P.S. Kalsi, New Age, 1996.
6. *Organic Chemistry Through Solved problems* by Goutam Brahmachari (Narosa Publishing House, New Delhi), ISBN: 978-81-7319-816-8, revised edition: 2014.