

Course Code	Course Name	Credits
26CH505	ORGANIC CHEMISTRY: STRUCTURE AND MECHANISMS	04

Course Objectives

- To understand the mechanisms and synthetic importance of oxidation and reduction reactions.
- To explain nucleophilic and electrophilic substitution reactions, including their mechanisms, stereochemistry, and influencing factors.
- To analyze elimination and esterification reactions and develop the ability to predict reaction pathways and products.

Learning Outcomes

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

- Understand oxidation and reduction reactions, their mechanisms, and synthetic applications in organic chemistry.
- Apply various reagents and methods for formation and cleavage of C–C and C=C bonds.
- Analyze nucleophilic and electrophilic substitution reactions, including mechanisms and influencing factors.
- Evaluate elimination reactions, esterification, and hydrolysis mechanisms with emphasis on reactivity and stereochemistry.

Unit 1 - Oxidation (12 Hrs.)

Mechanistic study of alcohol oxidation using Cr(VI) and manganese reagents; oxidation of methylene groups to carbonyl compounds; oxidation of aryl methanes; Etard reaction; allylic oxidation of olefins (including SeO₂ oxidation); oxidation of alcohols, glycols, halides and amines to aldehydes and ketones; oxidation of olefinic double bonds and unsaturated carbonyl compounds; oxidative cleavage of C–C bonds; formation of C=C bonds (Wittig reaction); formation of C–C bonds by dehydrogenation; dehydrogenation using quinones, Hg(OAc)₂ and Pb(OAc)₄; C–C bond formation by phenol coupling and acetylene coupling..

Unit 2 – Reduction (12 Hrs.)

Synthetic importance of Clemmensen and Wolff–Kishner reductions; modifications of Wolff–Kishner reduction; Birch reduction; Meerwein–Ponndorf–Verley (MPV) reduction; catalytic hydrogenation; reductions using LiAlH₄, NaBH₄, DIBAL-H, tri-tert-butoxyaluminium hydride, sodium cyanoborohydride, trialkyltin hydride, and hydrazine.

Unit 3 - Nucleophilic Substitution Reactions (12 Hrs.)

SN₁, SN₂, and SN_i mechanisms and their stereochemistry; neighbouring group participation; nucleophilic substitutions at aliphatic, allylic, and vinylic carbons; effect of substrate, nucleophile, leaving group, and solvent (medium) on nucleophilic substitution reactions; ambident nucleophiles; aromatic nucleophilic substitutions (S_NAr, S_N1, and benzyne mechanisms); Sommelet–Hauser, Von Richter, and Smiles rearrangements; Bucherer reaction and Rosenmund reduction.

Unit 4 – Electrophilic Substitution Reactions (12 Hrs.)

Aromatic electrophilic substitution—mechanism, reactivity, selectivity, and orientation; effect of substituents on electrophilic substitution reactions; nitration, nitrosation, diazonium coupling, sulphonation, chlorination and bromination; Friedel–Crafts alkylation, acylation, and arylation; aliphatic electrophilic substitution mechanisms (SE₁, SE₂, and SE_i); addition–elimination and cyclic mechanisms; halogenation of aldehydes, ketones, and carboxylic acids; aliphatic diazonium coupling; sulphonation, sulphenylation, and acylation; Stork enamine reaction; carbene and nitrene insertions; Kolbe–Schmitt reaction.

Unit 5 - Elimination and Esterification Reactions (12 Hrs.)

E₁, E₂, and E₁cB mechanisms; Hofmann and Saytzeff (Zaitsev) rules; syn versus anti-elimination; competition between elimination and substitution; factors influencing elimination and substitution reactions; dehydration, dehydrohalogenation, and dehalogenation; stereochemistry of E₂ elimination in cyclohexane systems; mechanism of pyrolytic eliminations (Chugaev and Cope eliminations); esterification and hydrolysis—mechanism of hydrolysis of esters, amides, and acyl halides; esterification of acids and transesterification.

Reference Books:

- J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 2001, Oxford University Press.
- M.B. Smith & J. March, March's Advanced Organic Chemistry, 5th Edn., 2001, John Wiley & Sons, New York.
- F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B, 2004, KluwerAcademic/Plenum Publishers, New York.

Websites and eLearning Sources:

- <http://www.digimat.in/nptel/courses/video/104101127/L16.html><https://nptel.ac.in/courses/104105086>
- <https://www.youtube.com/watch?v=68qMmO0F6uU>

COs and Bloom's Taxonomy Mapping – 26CH505		
Course Outcomes	On completing P.G. program the students will be able to	BTL
CO1	Define and explain mechanisms underlying oxidation- reduction, nucleophilic, electrophilic substitution and elimination processes.	K1, K2
CO2	Predict the outcome of the oxidation-reduction, substitution and elimination reaction when provided with the reactants and conditions.	K3
CO3	Differentiate different types of reactions, identifying the conditions that favor each mechanism.	K4
CO4	Assess the suitability of different reagents and conditions for achieving a specific organic transformation.	K5
CO5	Design synthetic pathways for complex molecules involving multiple steps.	K6

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

Relationship Matrix – 26CH505												
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	2	3	1	1	2	3	2	3	1	2	2.1
CO2	3	3	3	1	1	3	3	3	3	2	3	2.5
CO3	3	3	3	1	1	3	3	3	3	3	3	2.6
CO4	3	3	3	1	1	2	2	3	3	3	3	2.4
CO5	2	3	3	1	2	3	3	3	3	3	3	2.6
Total												2.4

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

