

Course Code	Course Title	C	H	I	E	T
17P1CMC1	ORGANIC CHEMISTRY-I	4	4	25	75	100

UNIT I NATURE OF BONDING IN ORGANIC MOLECULES 12 Hrs

Delocalized chemical bonding – conjugation - cross conjugation – resonance – hyperconjugation -bonding in fullerenes – tautomerism.

Aromaticity: Huckel rule- aromaticity, anti-aromaticity, homo aromaticity, in benzenoid and non-benzenoid compounds, alternant-non-alternant hydrocarbons, energy level of π -molecular orbitals, annulenes.

Bond weaker than covalent - addition compound, crown ethers, complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

UNIT II REACTION MECHANISM, STRUCTURE AND REACTIVITY 12 Hrs

Electronic effects-Inductive, field, Resonance-Steric Inhibition of Resonance.

Types of mechanisms- potential energy diagrams, transition states and intermediates- kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, hard and soft acids and bases.

The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Reactive Intermediates: Carbocation, carbanion, carbene and nitrene: generation, structure and reactivity-

UNIT III ALIPHATIC NUCLEOPHILIC SUBSTITUTION 12 Hrs

The S_N^1 , S_N^2 , mixed S_N^2 and S_N^i mechanisms.

The neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and non classical carbocations, phenonium ions, norbornyl system, common carbocation, rearrangements, applications of NMR spectroscopy in the detection of carbocations

The S_N^i mechanism. Nucleophilic substitution at allylic, aliphatic trigonal, vinylic carbon.

Effects of substrate structure, attacking nucleophile, leaving group, and solvent polarity on the reactivity.

UNIT IV AROMATIC ELECTROPHILIC AND NUCLEOPHILIC SUBSTITUTION

12 Hrs

The arenium ion intermediate, energy profile diagrams, orientation and reactivity in mono and disubstituted benzene ring - ortho/para ratio, ipso attack, orientation in other ring systems: naphthalene, anthracene, phenanthrene, pyrrole, indole, pyridine, quinoline and isoquinoline. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann –Koch reaction.

Aromatic Nucleophilic substitution: The S_NAr , S_N^1 and benzyne mechanisms. Reactivity-effect of substrate structure, leaving group and nucleophile. The Von Richter, Sommelet Hauser and Smiles rearrangements.

UNIT V FREE RADICAL AND ELIMINATIONS REACTIONS 12 Hrs

Types of free radical reactions, free radical substitution mechanism, mechanism at 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.

Allylic halogenation, oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Free radical rearrangement, Hunsdiecker reaction.

Elimination Reactions

The E₂, E₁ and E₁CB mechanism - Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. The mechanism and orientation of pyrolytic elimination.

Text Book(s):

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P., “Organic Chemistry”, First Edition, Oxford University Press, New York, 2006.
2. March, J., “Advanced Organic Chemistry”, Sixth Edition, John Wiley & Sons, New York, 2007.
3. Smith, M. B., “Organic Synthesis”, Second Edition, McGraw-Hill International Edition, New Delhi, 1994.
4. Skyes, P., “A Guide Book to Mechanism in Organic Chemistry”, Sixth Edition, Pearson Education Ltd., New Delhi, 2011.
5. Finar, I.L., “Organic Chemistry”, Vol. II, Sixth Edition, Pearson Education Pvt. Ltd., Singapore, 2006.
6. Mukherji, S.M., and Singh, S. P., Organic Reaction Mechanism by MacMillan India Ltd.

Reference Books:

1. Ahluvalia, V.K., “Chemistry of Natural Products”, First Edition, Vishal Publishing Co, Jalandhar, 2008.
2. Carrutherus, W., “Some Modern Methods in Organic Synthesis”, Third Edition, Cambridge University Press, New York, 1997.
3. Ireland, R.E., “Foundation of Modern Organic Chemistry Series- Organic Synthesis”, First Edition, Prentice – Hall of India Pvt. Ltd., New Delhi, 1975.
4. Mackie, R.K., Smith, M.M., and Aitken, R.A., “Guide Book to Organic Synthesis” Second Edition, Longman Scientific and Technical, Singapore, 1990.
5. Bruckner, R., “Advanced Organic Chemistry – Reaction Mechanism”, First Edition, Elsevier India Pvt. Ltd., New Delhi, 2005.
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