OC H 412: ORGANIC CHEMISTRY

Course Outcome

- Enable the students to learn the bonding in organic systems, various aspects of aromaticity, electronic effects, acidity and basicity of organic compounds.
- To gain knowledge on methods of determination of reaction mechanism, various reaction intermediates, aliphatic electrophilic and nucleophilic substitution reactions.
- To understand the detailed aspects of optical and geometrical isomerism.

UNIT-I **[12 Hours]**

Localized chemical bonding: Hybridization index, bonding in cyclopropane, bond distances, bond angles, bond energies, bond polarity, dipole moment and calculation of heat of reactions.

Delocalized chemical bonding: Conjugation, cross conjugation, resonance, steric inhibition of resonance, hyperconjugation, tautomerism, valence tautomerism. Bonding in fullerenes.

Bonding weaker than covalent: Hydrogen bonding, EDA complexes, inclusion compounds, Addition compounds, catenanes, rotaxanes and fluxional molecules.

Aromaticity: HMO theory and its application to simple π systems - ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl systems.

Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non benzenoid molecules - Tropones, tropolones, borazine and azulene. Annulenes & hetero-annulenes.

UNIT-II **[12 Hours]**

Organic Acids and bases: Brönsted-Lowry, Lewis concepts of organic acids and bases, pH, pKa values. Electronic (resonance, inductive and hyperconjugation), steric, hydrogen bonding and solvent effects on the strengths of acids and bases. HSAB concept.

Methods of Determining Reaction Mechanism: Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, kinetic evidences and kinetic isotopic effects. Limitation of reactions.

Reaction Intermediates: Generation, structure, stability, reactivity, detection, trapping and reactions of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules.

UNIT-III **[12 Hours]**

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions-S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions. Neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions.

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms - S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts. α-

halogenation of aldehydes and ketones, aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogen, mercury exchange reactions.

UNIT-IV: Stereochemistry **[12 Hours]**

Optical Isomerism: Conformation and configuration. Projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations, interconversion of projection formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, Psedoassymmetric centres. Racemizations and resolution methods. Stereospecific and stereoselective reactions. Asymmetric synthesis-Cram's and Prelog's rules. Optical activity in the absence of chiral carbon atom-biphenyls, allenes, spiranes, adamentanes, ansa compounds, cyclophanes, *trans*-cyclooctene, binaphthyls, catenanes, rotaxanes, and helicenes. Conformational analysis of cycloalkanes and decalins.

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers.

References

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