Subject Code : P8CH1

CORE COURSE I - ORGANIC CHEMISTRY I

UNIT – I

1. Structure and Bonding

Nomenclature of alicyclic, bicyclic and tricyclic compounds. (Basic skeletal structures only with or without one substituent)

Localized Chemical Bonding: Electronic Structure of molecules; VB, MO and HOMO-LUMO theory, Electronegativity, Dipole Moment, Inductive and Field Effects, Bond distances, Bond angles, Bond energies.

Delocalized Chemical Bonding: Bond energies and Bond distances in compounds containing delocalized Bonds, Cross conjucation, Resonance, Steric inhibition of resonance, Hyperconjugation, Keto – Enol Tautomerism.

2. Acids and Bases

Bronsted theory – Lewis acids and bases – Effect of structure on the strengths of acids and bases.

UNIT – II

3. Aromaticity

Aromatic character: six-, Five-, seven-, and eight-membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, Concept of homoaromaticity and antiaromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems of more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with $(4n + 2)\pi$ electrons and $4n\pi$ electrons, Heteraromatic molecules. Annulenes and sydnones and fullerenes.

4. Heterocycles

Nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Synthesis, reactivity and applications of the following heterocycles: Pyrazoles, Oxazoles, Pyridazines, Pyrimidine and Pyrazines.

UNIT- III

5. Stereochemistry

Fundamentals of Organic Stereochemistry: Principles of symmetry – Stereoisomerism – Optical isomerism - Definitions – Conventions used in stereochemistry: Newman, Sawhorse and Fischer notations and interconversions and representations. Nomenclature, correlation of configuration. Cahn – Ingold – Prelog rules for simple molecules. Optical activity and chirality – Types of molecules exhibiting optical activity – Fischer projection – Absolute configuration. Molecules with more than one chiral centre – Molecular chirality – Atropisomerism – Biphenyls, allenes and spiranes. Methods of determining configuration. Enantiomerism of compounds containing chiral heteroatoms – Walden inversion – Asymmetric synthesis based on Cram's rule – Enantiotopic behaviour and Prochiral centres.

6. Geometrical Isomerism

E & Z Nomenclature, Determination of configuration of geometrical isomers, Stereochemistry of addition and elimination reactions. Stereospecific and stereoselective synthesis – [Elementary examples].

7. Conformational Analysis

Basic concepts of conformational analysis – Conformations of *n*-butane, cyclohexane and decalins.

UNIT IV

8. Organic Photochemistry

Organic Photochemistry – Fundamental concepts – Jablonski diagram – Energy transfer, characteristics of photoreactions, photoreduction and photoxidation, photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds, reactions of unactivated centres – Photolytic cycloadditions and photolytic rearrangements – Photosenstitisation – Photoadditions – Barton reaction – Parterno Buchi reaction.

UNIT V

9. Reactive Intermediates

Carbocations, Carbanions, Carbenes and Nitrenes – Generation and stability of reactive intermediates. Correlation of reactivity with structure of reactive intermediates. Free radicals – Configurations – Identification by chemical and spectral methods – Free radical halogenation - NBS.

10. Methods of Determining Reaction Mechanisms

Types of reactions: Homolytic and Heterolytic cleavages of bonds, Characteristics of nucleophilic, electrophilic and free radical reactions. Thermodynamic and kinetic aspects, Hammond's postulate, isotope effects. Energy profile diagrams – Intermediate versus transition state, Product analysis and its importance, Crossover experiments, Kinetic methods, Stereochemical studies, Isotopic and substitutent effects.

References

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5thed.,Wiley, 2000.
2. D. Nasipuri, Stereochemistry of organic compounds-Principles and applications, New Age International, 2ndEdition,2002.
3. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.
4. R.K. Bansal, Organic Reaction Mechanisms, Tata McGraw Hill, 1975.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th ed., Pearson, 1992.
6. J.D. Coyle, Organic Photochemistry - Wiley, 1985.
7. J.M. Coxon, B. Halton, Organic Photochemistry, Camb. Uni. Press, 2nd edition, 1987.
8. G.R. Chatwal , OrganicPhtochemistry, Himalaya Publications house, 1st edition, 1998.
9. P.S. Kalsi, Stereochemistry , Wiley eastern limited, New Delhi, 1990.