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- 6. R.A. Day and A.L. Underwood: Quantitative Analysis, 5th Ed. (Prentice Hall, India), 1998.

AC H 402: 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 and aliphatic nucleophilic substitution reactions.
- To understand the detailed aspects of optical and geometrical isomerism.

UNIT–I: [15 Hours]

Bonding in organic systems: Theories of bonding-Valence and molecular orbital approaches. Resonance, hyper-conjugation and tautomerism, Huckel molecular orbital theory and its application to simple systems- ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, heptatrienyl systems. Calculation of the total energy and M.O. coefficients of the systems. 5 hrs

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, Homo-aromatic, non aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes & hetero-annulenes. Physical methods to study aromaticity-UV, IR & H NMR.

4 hrs

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules.

3 hrs

Structure and reactivity: Effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

3 hrs

UNIT-II: [15 Hours]

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical

evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects.

5 hrs

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. 5 hrs **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, Walden inversion, neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions.

UNIT-III: Stereochemistry

[15 Hours]

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations. Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

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. 3 hrs

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- 2. Stereochemistry, Conformation and Mechanism-P.S. Kalsi (Wiley Eastern, New Delhi) 1993.
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- 6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
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