

SEMESTER - III

Course III (ORGANIC CHEMISTRY & SPECTROSCOPY) 60hrs (4 h / w)

ORGANIC CHEMISTRY

34h

UNIT – I

1. Chemistry of Halogenated Hydrocarbons:

6h

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions— S_N1 , S_N2 and S_Ni mechanisms with stereo chemical aspects and effect of solvent etc.; nucleophilic substitutions. elimination, Williamson's synthesis. Aryl halides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; S_NAr , Benzyne mechanism. Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

2. Alcohols & Phenols

6h

Alcohols: preparation, properties and relative reactivity of 1° , 2° , 3° alcohols, Bouvaelt Blanc Reduction; Oxidation of diols by periodic acid and lead tetra acetate, Pinacol-Pinacolone rearrangement;
Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer-Tiemann and Kolbe's-Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

UNIT-II

Carbonyl Compounds

10h

Structure, reactivity, preparation and properties; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives
Mechanisms of Aldol and Benzoin condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann haloform reaction and Baeyer Villiger oxidation, α -substitution reactions, oxidations and reductions (Clemmensen, wolf-kishner, with $LiAlH_4$ & $NaBH_4$). Addition reactions of α , β -unsaturated carbonyl compounds: Michael addition.
Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

UNIT-III

Carboxylic Acids and their Derivatives 12h

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituents on acidic strength. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids. Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group-Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Reformatsky reactions and Curtius rearrangement Reactions involving H, OH and COOH groups- salt formation, anhydride formation, acid chloride formation, amide formation and esterification (mechanism). Degradation of carboxylic acids by Hunsdiecker reaction, decarboxylation by Schmidt reaction, Arndt-Eistert synthesis, halogenation by Hell- Volhard- Zelinsky reaction.

SPECTROSCOPY

26 h

UNIT-IV

Molecular Spectroscopy:

18h

Interaction of electromagnetic radiation with molecules and various types of spectra;

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, Harmonic and anharmonic oscillator, Morse potential curve, vibrational degrees offered for polyatomic molecules, modes of vibration. Selection rules for vibrational transitions, Fundamental frequencies, overtones and hot bands.

Electronic spectroscopy: Energy levels of molecular orbitals (σ , π , n). Selection rules for electronic spectra. Types of electronic transitions in molecules, effect of conjugation. Concept of chromophore. bathochromic and hypso chromic shifts. Beer-Lambert's law and its limitations.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of nuclear magnetic resonance, equivalent and non-equivalent protons, position of signals. Chemical shift, NMR splitting of signals - spin-spin coupling, coupling constants. Applications of NMR with suitable examples - ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromo ethane, ethyl acetate, toluene and acetophenone.

UNIT-V

8h

Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules.

Application of electronic spectroscopy and Woodward rules for calculating λ_{\max} of conjugated dienes and α , β – unsaturated compounds. Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on $>C=O$ stretching absorptions).

List of Reference Books

1. A Text Book of Organic Chemistry by Bahl and Arunbahl
2. A Text Book of Organic chemistry by I L Finar Vol I
3. Organic chemistry by Bruice
4. Organic chemistry by Clayden
5. Spectroscopy by William Kemp
6. Spectroscopy by Pavia
7. Organic Spectroscopy by J. R. Dyer
8. Elementary organic spectroscopy by Y.R. Sharma
9. Spectroscopy by P.S.Kalsi
10. Spectrometric Identification of Organic Compounds by Robert M Silverstein, Francis X Webster
11. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
12. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012)
13. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

LABORATORY COURSE -III

30hrs (2 h / w)

Practical Course-III Organic preparations and IR Spectral Analysis

(At the end of Semester- III)

Organic preparations:

40M

i. Acetylation of one of the following compounds:

amines (aniline, o-, m-, ptoluidines and o-, m-, p-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:

a. Using conventional method.

- b. Using green approach
- ii. Benzoylation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine)
- iii. Nitration of any one of the following:
 - a. Acetanilide/nitrobenzene by conventional method
 - b. Salicylic acid by green approach (using ceric ammonium nitrate).

IR Spectral Analysis

10M

IR Spectral Analysis of the following functional groups with examples

- a) Hydroxyl groups
- b) Carbonyl groups
- c) Amino groups
- d) Aromatic groups