DEPARTMENT OF CHEMISTRY

SEMESTER - III

SYLLABUS

SEMESTER - III

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

Course outcomes:

At the end of the course, the student will be able to;

1. Understandpreparation,propertiesandreactionsofhaloalkanes,haloarenesand oxygencontaining functionalgroups.
2. Usethesyntheticchemistrylearntinthiscoursetodofunctionalgroup transformations.
3. Toproposeplausiblemechanismsforanyrelevantreaction

ORGANIC CHEMISTRY 34h

UNIT – I

1. Chemistry of Halogenated Hydrocarbons: 6h

Alkylhalides:Methodsofpreparationandproperties,nucleophilicsubstitutionreactions– SN1,SN2andSNimechanismswithstereochemicalaspectsandeffectofsolventetc.;nucleophilics ubstitutionvs. elimination, Williamson's synthesis.

Arylhalides:Preparation(includingpreparationfromdiazoniumsalts)andproperties,nucleophilic aromatic substitution;SNAr,Benzynemechanism.

Relativereactivityofalkyl,allyl,benzyl,vinylandarylhalidestowardsnucleophilicsubstitut ionreactions.

2. Alcohols &Phenols 6h

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, BouvaeltBlanc Reduction; Oxidationofdiolsbyperiodicacidandleadtetra acetate,Pinacol-Pinacolonerearrangement;

Phenols:Preparationandproperties;Acidityandfactorseffectingit, Ringsubstitution reactions, Reimer–Tiemannand Kolbe's–Schmidt Reactions, Fries and Claisenrearrangements with mechanism;

UNIT-II

CarbonylCompounds 10h

Structure,reactivity,preparationandproperties;

Nucleophilicadditions,Nucleophilicaddition-eliminationreactionswithammoniaderivatives MechanismsofAldolandBenzoincondensation, Claisan-Schmidt, Perkin, CannizzaroandWittigreaction,Beckmannhaloformreactionand BaeyerVilligeroxidation,α-

substitutionreactions,oxidationsandreductions(Clemmensen, wolf –kishner, with LiAlH4 &NaBH4).

Additionreactionsof α,β-unsaturatedcarbonylcompounds:Michaeladdition.

Activemethylenecompounds: Keto-enoltautomerism.Preparationandsyntheticapplicationsofdiethyl malonateandethylacetoacetate.

UNIT-III

CarboxylicAcidsand their Derivatives **12h**

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituentsonacidicstrength.Typicalreactionsofdicarboxylicacids,hydroxyacidsandunsaturatedacids.

Preparationandreactionsofacidchlorides,anhydrides,estersandamides; Comparative study of nucleophilic substitutionatacyl group-Mechanism of acidicandalkaline hydrolysis of esters, Claisencondensation, Reform at sky 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 Huns-Diecker reaction, decarboxylation by Schimdt reaction, Arndt-Eistert synthesis, halogenation by Hell- Volhard- Zelinsky reaction.

SPECTROSCOPY **26 h**

UNIT-IV

Molecular Spectroscopy: **18h**

Interactionofelectromagneticradiationwithmoleculesandvarioustypesof 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, Morsepotential curve, vibrational degrees offered for polyatomic molecules, modesofvibration. 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 hypsochromic 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).

Co-curricular activities and Assessment Methods Continuous Evaluation: Monitoring the progress of student'slearning Class Tests, Work sheets and Quizzes Presentations, Projects and Assignments and Group Discussions: Enhances critical thinking skills and personality Semester-end Examination: critical indicator of student's learning and teaching methods adopted byteachers throughout the semester.

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 FinarVol 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-IIIOrganic preparations and IR Spectral Analysis

(At the end of Semester- III)

Course outcomes:

Onthecompletionofthecourse,thestudentwillbe abletodothefollowing**:**

1. how to use glassware, equipment and chemicals and follow experimental procedures in the laboratory
2. how to calculate limiting reagent, theoretical yield, and percent yield
3. how to engage in safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents appropriately
4. how to dispose of chemicals in a safe and responsible manner
5. how to perform common laboratory techniques including reflux, distillation, recrystallization, vacuum filtration.
6. how to create and carry out work up and separation procedures
7. how to critically evaluate data collected to determine the identity, purity, and percent yield of products and to summarize findings in writing in a clear and concise manner

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. Benzolyation 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

MODEL PAPER

SECOND YEAR B.Sc., DEGREE EXAMINATION

SEMESTER-III

CHEMISTRY COURSE-III: ORGANIC CHEMISTRY & SPECTROSCOPY

Time: 3 hours Maximum Marks: 75

PART- A 5 X 5 = 25 Marks

Answer any **FIVE** of the following questions. Each carries **FIVE** marks

1. Discuss two methods for preparation of aryl halides.
2. Explain the mechanism for Pinacol-Pinacolone rearrangement.
3. Discuss the mechanism for Bayer-villiger oxidation reaction.
4. Explain the effect of substituents on acidic strength of mono-carboxylic acids.
5. Write the mechanism for Claisen Condensation reaction.
6. Write the selection rules in rotational spectroscopy.
7. Explain Spin – Spin coupling and Coupling Constant.
8. Explain types of electronic transitions in UV spectroscopy.

PART- B 5 X 10 = 50 Marks

Answer **ALL** the questions. Each carries **TEN** marks

9 (a). Give the mechanism & stereochemistry of SN^1& SN^2 reactions of alkyl halides with suitable example.

(or)

(b). Explain the following reactions with mechanism.
(i) Reimer-Tiemann reaction (ii) Fries rearrangement.

10 (a). Discuss the mechanism for following reactions.
(i) Perkin reaction. (ii) Cannizaro reaction

(or)

(b). Write the preparation and any three synthetic applications of diethyl malonate.

11.(a). Explain acid and base hydrolysis reaction of esters with mechanism.

(or)

(b). Explain the mechanisms of Curtius rearrangement & Arndt –Eistert reaction.

12.(a). (i) Write a note on vibrational degrees of freedom for polyatomic molecules.
(ii) Explain different modes of vibrations & selection rules in IR spectroscopy.

(or)

(b).(i) Define Bathochromic shift. Explain the effect of conjugation in U.V. spectroscopy.
(ii) Discuss the principle of NMR spectroscopy.

13.(a). Write Woodward-Fieser rules for calculating λmax for conjugated dienes and α,β – unsaturated carbonyl compounds , and apply them for one example each.

(or)

(b).(i) What is Fingerprint region. Explain its signigicance with an example.(ii) Write IR spectral data for any one alcohol, aldehyde and ketone