P.B. SIDDHARTHA COLLEGE OF ARTS & SCIENCE

Siddhartha Nagar, Vijayawada – 520 010

Autonomous - ISO 9001 – 2015 Certified

Title of the Paper (ORGANIC CHEMISTRY & SPECTROSCOPY)
Course Code: 22CHET31

Offered to: II B.Sc MPC & BZC **Course Type :** Core (TH)

Year of Introduction: 2021 **Year of offering: 2021**

Year of Revision: 2021-22 **Percentage ofRevision: 5 %**

Semester: III **Credits: 4**

Hours Taught: 60 hrs. Per Semester **Max.Time**: 4Hours

Course Prerequisites (if any): 22CHET21

Course Description: Topics will include structure, stereochemistry, nomenclature, synthesis, properties, and reactions of the major classes of organic compounds. A mechanistic approach is used in the course to explain the reactions of these compounds.

Spectroscopy is general term used for the instrumental process by which information about molecular structure is obtained through careful analysis of absorption, scattering or emission of electromagnetic radiation by compounds.

Course Objectives:

1. Student will know the preparation, properties and reactions of halo alkanes, halo arenes and oxygen containing functional groups
2. Student Use the synthetic chemistry learnt in this course to do functional group transformations.
3. Will know the different types of carboxylic acids their preparations & properties
4. Knowing various applications of spectroscopy methods
5. Learn to apply spectroscopy to simple organic compounds

Course Outcomes: At the end of this course, students should be able to:

CO1: Remember the preparations, properties and reactions of halo alkanes, halo arenes and oxygen containing functional groups.-**PO1**

CO2: Understand preparation, properties and reactions of carbonyl compounds -**PO1**

CO3: Apply preparation methods for carboxylic acids and their derivatives-**PO1**

CO4: Analyze various molecules and polyatomic molecules using different spectroscopy methods-**PO1, PO7**

CO5: Evaluate the functional groups of different organic compounds- **PO1, PO7**

CO6: Create applications of spectroscopy for various organic molecules- **PO1, PO7**

Syllabus

Course Details

Unit	Learning Units	Lecture Hours
I	**Chemistry of Halogenated Hydrocarbons 6H** Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions– SN1, SN2 and SNi mechanisms with stereo chemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination, Williamson's synthesis. Arylhalides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; SNAr,	**12 Hrs**

	Benzyne mechanism. Relative reactivity of alkyl, allyl, benzyl,vinyl and aryl halides towards nucleophilic substitution reactions. **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; **Lucas Reagent** Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemannand Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;	
II	**Carbonyl Compounds** Structure, reactivity, preparation and properties; Nucleophilic additions, **with $NaHSO_3$, Formation of alcohols, HCN , Grignard's Reagent(Rmgx), hemi acetol's, Fehling's, Tollen's, 2 4 Di Nitro Phenyl hydrazine (2 4 DNPH) and formation of oximes** Nucleophilic addition-elimination reactions with ammonia derivatives Mechanisms of Aldol and Benzoin condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann halo form reaction and Baeyer Villiger oxidation, α- substitution reactions,oxidations and reductions (Clemmensen, wolf – kishner, with LiAlH4 & NaBH4). Addition reactions of α,β-unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto- Enolt automerism. Preparation and synthetic applications of diethyl malonate and ethyl aceto acetate.	**10 hrs**
III	**Carboxylic Acids and their Derivatives** General methods of preparation, physical properties and reactions of mono carboxylic acids, effect of Substituents on acidic strength.Typical reactions of dicarboxylic acids, hydroxyl 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, 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, de carboxylation by Schimdt reaction, Arndt- Eistert synthesis, halogenation by Hell- Volhard- Zelinsky reaction.	**12 hrs**
IV	**Molecular Spectroscopy**: 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 an harmonic oscillator, Morse potential curve,vibrational degrees of freedom molecules, modes of vibration. Selection rules for vibrational transitions, Fundamental frequencies, overtones and hotbands. **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.	**18 hrs**
V	**Application of Spectroscopy to Simple Organic MoleculesApplication 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).	**8 hrs**

Textbook:

1. B.S.Bhal, Arun Bhal Advanced Organic Chemistry, Ramnagar, New Delhi 2001
2. P K Bruice. Organic Chemistry by Bruice, Pearson Education, Patparganj, Delhi-2001
3. Jonathan Clyden, Nick Greaves, Oganic Chemistry by Clyden, Oxford University press
4. William Kemph, Spectroscopy by William Kemp, Palgrave, USA-3rd edition
5. Y R Sharma, Elementary Organic Spectroscopy, S Chand, 4th revised edition.

Recommended Reference book:

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. &Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

Course Delivery method: Face-to-face / Blended

Course has focus on:

Employability / **E**ntrepreneurship

Websites of Interest:

1. **https://www.sydney.edu.au/science/chemistry/~george/halides.html**
2. **https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_(McMurry)/17%3A_Alcohols_and_Phenols/17.00%3A_Introduction**
3. **https://nptel.ac.in/content/storage2/courses/104101005/downloads/LectureNotes/chapter%2010.pdf**
4. **https://www.khanacademy.org/science/organic-chemistry/carboxylic-acids-derivatives/formation-carboxylic-acid-derivatives-sal/v/fisher-esterification?modal=1**
5. **https://byjus.com/chemistry/infrared-spectroscopy/**
6. **https://www.lehigh.edu/~kjs0/carey-13.PDF**

Co-curricular Activities:

Continuous Evaluation: Monitoring the progress of student's learning Class Tests Work sheets and Quizzes Presentations, Assignments and Group Discussions.

MODEL PAPER FOR INTERNAL EXAMINATION

Max. Marks: 30 **Max.**

Time: 90min

Answer all Questions. All questions carry equal marks.

(Restrict to a maximum of 2 subdivisions)

Unit -I

1.	(a)	(i)	10M	L1
			OR	
		(ii)	10M	L1
	(b)	(i)	5 M	L2
			OR	
		(ii)	5 M	L2

Unit –II

2.	(a)	(i)	10M	L3
			OR	
		(ii)	10M	L3
	(b)	(i)	5 M	L2
			OR	
		(ii)	5 M	L2

SEMESTER END EXAMINATION MODEL PAPER
SEMESTER-III
CHEMISTRY COURSE-III: ORGANIC CHEMISTRY & SPECTROSCOPY

Time: 3 hours Maximum Marks: 70

PART- A

5 X 4 = 20Marks

Answer the following questions. Each carries **FOUR** marks

1. a)Tell any two methods for preparation of aryl halides- **L1-CO1**

Or

b) Summarize the mechanism for Pinacol-Pinacolone rearrangement L1 CO1

2. a)Summarize the mechanism for aldol condensation -**L2-CO2**

Or

b). Interpret the mechanism for Bayer-villiger oxidation reaction.-**L2-CO2**

3. a)Explain the effect of substituents on acidic strength of mono-carboxylic acids.-**L1-CO3**

Or

b) Explain the mechanism for Claisen Condensation reaction. **L1-CO3**

4. a)Tell the selection rules in rotational spectroscopy.-**L1-CO4**

Or

b). Explain Spin – Spin coupling and Coupling Constant.-**L1-CO4**

5.a) Classify types of electronic transitions in UV spectroscopy.**L2- CO5**

Or

b) Summerize Fingerprint region and its significance with an example.L1 CO5

PART- B

5 X 10 = 50 Marks

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

9 (a). Explain the mechanism & stereochemistry of SN1& SN2 reactions of alkyl halides with suitable example.**L1-CO1**

(or)

(b). Explain the following reactions with mechanism. **L1-CO1**
(i) Reimer-Tiemann reaction (ii) Fries rearrangement.

10 (a). Interpret the mechanism for following reactions.**L2-CO2**
(i) Perkin reaction. (ii) Cannizaro reaction

(or)

(b). Summarize the preparation and any three synthetic applications of diethyl malonate.**L2-CO2**

11. (a). Explain acid and base hydrolysis reaction of esters with mechanism. **L1-CO3**

(or)

(b). Explain the mechanisms of Curtius rearrangement & Arndt –Eistert reaction.**L1-CO3**

12. (a). (i) Tell a note on vibrational degrees of freedom for polyatomic molecules.**L1-CO4**
(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.**L1-CO4**
(ii) Describe the principle of NMR spectroscopy.

13. (a). Relate Woodward-Fieser rules for calculating λmax for conjugated dienes and α,β – unsaturated carbonyl compounds , and apply them for one example each. **L2-CO5**

(or)

(b). Summrize the IR spectral data for any one alcohol, aldehyde and ketone –**L2-CO5**

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Title of the Paper (ORGANIC PREPARATIONS AND IR SPECTRAL ANALYSIS)

Course Code:22CHEL31

Offered to: II B.Sc MPC & BZC **Course Type :** Core (Pr)

Year of Introduction: 2021 **Year of offering: 2021**

Year of Revision: 2021-22 **Percentage of Revision:**

Semester: III **Credits: 1**

Hours Taught: 30 hrs. Per Semester **Max.Time** : 2 Hours

Course Prerequisites (if any): Basics of Organic Preparations and IR Spectroscopy

Course Description: Preparation of different organic compounds using conventional, Green approach methods and IR spectral analysis for different functional groups

Course Objectives:

1. Student will know the safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents appropriately.
2. Dispose of chemicals in a safe and responsible manner
3. Create and carry out work up and separation procedures

Course Outcomes: At the end of this course, students should be able to:

CO1: How to calculate limiting reagent, theoretical yield, and percent yield

CO2: How to perform common laboratory techniques including reflux, distillation, recrystallization, vacuum filtration.

CO3: 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

Syllabus

Course Details

Unit	Learning Units	Practical Hours
I	**Organic preparations:** 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).	**20 Hr**
II	**IR Spectral Analysis** IR Spectral Analysis of the following functional groups with examples a) Hydroxyl groups b) Carbonyl groups	**10Hr**

	c) Amino groups d) Aromatic groups	

Text Book
Laboratory Manual

Course Delivery method: Demonstration of Practical

Course has focus on:
Employability / **E**ntrepreneurship

MODEL PAPER

SECOND YEAR B.Sc., DEGREE EXAMINATION

SEMESTER-III

ORGANIC PREPARATIONS AND IR SPECTRAL ANALYSIS

22CHE L31

Total Marks: 50M

Part-I
Internal continuous Assessment - 15Marks

Part-II
Semester end exam - 35Marks