VANITA VISHRAM WOMEN'S UNIVERSITY

SCHOOL OF SCIENCE AND TECHNOLOGY

DEPARTMENT OF CHEMISTRY

SEMESTER 4

Core Courses (CC), Department Specific Elective (DSE)

Syllabus applicable to the students seeking admission in the following programmes

M.Sc. Organic Chemistry under LOCF

w.e.f. the Academic Year 2022-2023

1. Preamble – VVWU

Vanita Vishram Women's University (VVWU) is the First-ever Women's University of Gujarat approved by the Government of Gujarat under the provisions of the Gujarat Private Universities Act, 2009. It is a University committed to achieve Women's Empowerment through Quality Education, Skill Development, and by providing employment opportunities to its girl students through its model curriculum, integration of technology in pedagogy and best-in-class infrastructure. The focus is on prioritizing practical component and experiential learning supported through academia-industry linkages, functional MoUs, skill development training, internships etc. It aims at providing opportunities to the girl students for holistic development and self-reliance.

VISION

Empowerment of women through quality education and skill development, so as to make them strong pillars of stability in the society.

MISSION

To provide Education & Professional Training to all women for their all-round development, so as to enable them to become economically independent and socially empowered citizens.

SEMESTER 4
CORE COURSE

Selected Topics in Organic Chemistry (CH21220)

(Credit 4+1)

Course objective:

- Learn the important aspects Mass spectrometry and their applications
- Reaction mechanism involves different radicals.
- Understand the important aspects of Structure-Reactivity Principles for better understanding of reaction mechanism
- Classification, structure, mechanism of reactions of few selected Vitamins and Terpenoids.
- To understand the nomenclature of Heterocyclic molecules.
- To learn the importance of Heterocyclic Compounds in preparation of industrially important compounds.

Prerequisite:

- Basic knowledge of spectroscopic principles.
- Fundamental of heterocyclic chemistry.
- Basic terms and fundamental aspects related to Vitamins and Terpenoids.
- Pharmaceutics/Biomedical applications of Vitamins and Terpenoids.
- General classification and fundamentals of Terpenoids.
- Chemical kinetics in organic chemistry.
- Electrophilic and nucleophilic substitution reactions.
- Concepts of aromaticity.

Unit-I Mass Spectrometry (MIB)

Theory and principles of mass spectroscopy; Instrumentation; Ionization techniques – Electron Impact (EI) ionization, Chemical Ionization (CI), etc; Determination of molecular weight and molecular formula, nitrogen rule, detection of molecular ion peak, metastable ion peak; Fragmentations – rules governing the fragmentations, McLafferty rearrangement; Interpretation of mass spectra of different class of compounds, To write possible fragmentation for given compound; To identify structure from mass spectral data.

Unit-II Heterocyclic Chemistry(SDM)

Nomenclature of heterocycles: Hantzsch Widman System of Monocyclic, Fused heterocyclic, spiro and bicyclic. Five and six membered heterocycles with more than two hetero atoms: Synthesis, reactivity, aromatic character and importance of following heterocycles: triazoles, oxadiazoles. Condensed six membered heterocycles: Synthesis, reactivity, aromatic character and importance of following heterocyclic Rings: Cinnoline, Quinoxaline, Phthalazine, Naphthyridine, Phenoxazine.

Unit-III Structure-Reactivity Principles (NP)

Types of mechanisms, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtian-Hammet principle, potential energy diagrams, transition state and intermediates, methods of determining mechanisms, isotope effect. Effect of structure on reactivity- resonance and field effect, steric effect, quantitative treatment. The Hammet equation and linear free energy relationships, substituent and reaction constants, positive and negative deviation from Hammet equation, Taft equation, Solvent effect.

Unit-IV Vitamins & Terpenoids (SS)

(A) Vitamins Structure determination, Synthesis and biochemical functions of Vitamin A, Vitamins B1 and B2, Vitamin H
(B) Terpenoids Classification, nomenclature and isolation Structure determination and synthesis of Farnesol, Zingiberene, Cadinene, Gibrelic acid and Abietic acid.

Learning outcomes:

- It will increase their conceptual base and understanding of Structural elucidation using spectroscopy.
- Understand the knowledge of heterocyclic chemistry in organic chemistry allied branches.
- Able to apply the knowledge of structure reactivity principles in organic chemistry allied branches.
- In depth understanding of vitamins and their structures.
- To understand the synthesis of terpenoids.

Reference Books:

1. Spectroscopic Identification of Organic Compounds, R. M. Silverstein and F. X. Webster, 6th edition (John Wiley & Sons).
2. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rdedition (Thomson Brooks/Cole).
3. Organic Spectroscopy – Principles and Applications, Jag Mohan, 2nd edition (Narosa Publishing House)
4. Elementary Organic Spectroscopy: Principles and Chemical applications (revised edition), Y. R. Sharma (S. Chand Publishing)
5. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers
6. Heterocyclic Chemistry- J A Joule and Smith.
7. Heterocyclic Chemistry-II- R R Gupta, M Kumar, V Gupta, Springer (India) pvt.
8. Heterocyclic Chemistry, 3rd Edition by Thomas L. Gilchrist, Published by Prentice Hall (1997).
9. Heterocyclic chemistry by V. K. Ahluwalia, Narosa publishing house.

10. Topics in Heterocyclic Chemistry. G. W. Gribble. Springer-Verlag, Berlin Heidelberg, 2010.
11. Modern Heterocyclic Chemistry. 4 Volume Set. Julio Alvarez-Builla, Juan Jose Vaquero, José Barluenga. Wiley. 2011.
12. Chemistry of Organic Natural Products, Vol. I & II, O. P. Agrawal.
13. Chemistry of Vitamins – S. F. Dyke.
14. Chemistry of Natural Products, N. R. Krishnaswamy.

CORE COURSE

Modern Organic Reactions (CH21230)

(Credit 4+1)

Course objective:

- Chemistry of Palladium catalyzed the Carbon-carbon coupling reaction and its applications.
- Applications of carbene and metathesis reactions.
- Understand the general strategy of asymmetric synthesis and the classification into chiral substrate, auxiliary, reagent and catalyst controlled processes.
- Be able to give a detailed account of the course and mechanism of illustrative examples of the following asymmetric reactions that utilize chiral auxiliaries: enolate alkylation (oxazolidinones, oxazolines and chiral hydrazones), asymmetric (Evans) Aldol reaction and cycloaddition.
- To learn the radical reactions.
- To understand the importance of molecular rearrangement in organic transformation.
- Role of rearrangement reactions in the preparation of industrially important compounds.

Prerequisite:

- General group transformation reaction.
- Chemistry of carbene and general preparations.
- Basics of radical formation reaction.
- the specification of absolute and relative configuration and the measurement of the selectivity of stereoselective reactions.
- Basic idea about Rearrangement.

Unit-I Coupling Reaction(NJC)

Transition metals form organic compounds, The structure of σ and π complexes and the meaning of η numbers, The bonding is described with the usual orbitals, Most stable complexes have 18 valence electrons, Metals catalyze ‘impossible’ reactions, Oxidative insertion, reductive elimination, and ligand migration from metal to carbon are key steps, Carbon monoxide inserts into metal–carbon bonds, Palladium is the most important metal, C–C, C–O, and C–N bonds can be made with Pd catalysis, Cross-coupling of two ligands is common, Allyl cation complexes are

useful electrophiles, cross coupling reactions (Heck reaction, Suzuki, Stille, Negishi, Kumada, Hiyama, Sonogashira, Buchwald-Hartwig).

Unit-II Rearrangement reactions(SDM)

Rearrangement of Carbocations, Carbene, Nitrene, Dienone–phenol, Favroskii, Benzil-Benzilic acid, Schmidt, Lossen, Hoffman Reaction, Curtius, Beckmann, Neber, Payne, Sommelet–Hauser, Wittig, Rupe rearrangement, Smiles, Jacobsen, Orton.

Unit-III Radical reactions(NP)

Radicals contain unpaired electrons, Radicals form by homolysis of weak bonds, Most radicals are extremely reactive, analyze the structure of radicals: electron spin resonance Radical stability, radicals reaction, Radical–radical reactions, Radical chain reactions, Chlorination of alkanes, Allylic bromination, Reversing the selectivity: radical substitution of Br by H Carbon –carbon bond formation with radicals, the reactivity pattern of radicals is quite different from that of polar reagents, Alkyl radicals from boranes and oxygen, Intramolecular radical reactions are more efficient than intermolecular

Unit-IV Asymmetric Synthesis(SS)

Concise introduction to asymmetric synthesis, detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and Organo catalysts with specific examples. Chiral auxiliaries in asymmetric alkylation and aldol reactions, Chirality derives from nature, Chiral catalysts for oxidation and reduction reactions, Ligand-accelerated catalysis, Catalysis with and without metals

Reference Books:

1 G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006
2 B. M. Trost and I Fleming, Comprehensive organic synthesis, Pergamon Press, 1992.
3 Organometallics in Organic Synthesis, J. M. Swan, D. St. C. Black, Chapman and Hall, London, 1974
4 Organotransition Metal Chemistry: Applications to Organic Synthesis, S. G. Davis, Pergamon Press, Oxford, 1982.
5 Basic Organometallic Chemistry, B. D. Gupta, A J Elias, Universities Press, Chennai, 2010
6 Transition Metals in the total synthesis of complex organic molecules, L. S. Hegedus, University Science Books, 1994.

Course Outcome:

- To understand the application of asymmetric synthetic methods, in the total syntheses of important and complex chiral compounds.
- To understand the importance of rearrangement reactions in FGI.
- To learn the concept of coupling reactions.

Organic Chemistry Practical (CH21240)

(Credit 4)

Course objective:

- To introduce and practice various softwares used for data handling and data sorting.
- To gain an understanding of how to use different softwares for chemical structure drawing.
- To gain an understanding of how to use different softwares for chemical structure determination.

Prerequisite:

- Basic knowledge of operating computers.
- Able to handle basic softwares and working of computers.
- To be familiar with typing and browsing.
- General understanding of internet surfing and information of selective useful websites for chemistry.

Practicals to be performed:

1. Origin Software for data handling and presentation.
2. Computer Softwares based on MS Office: MS Word, MS Power Point, MS Excel data sheets creation, and tables using Excel Programme.
3. Exposure to available standard application packages like: Chemsketch, Chemdraw.
4. Literature Survey form various databases (i.e. Scopus)

Course Outcome:

- Able to apply knowledge of various softwares for better data analysis and data presentation.
- Will be able to handle and manage data to generate graphical presentations.

DSE Departmental Specific Elective-III

Material Nano Science (Credit 3+1)

(CH24080)

Course objective:

- The objective of the course is to provide basic knowledge on surface science
- To prepare the student to understand a series of phenomena relevant colloids and soft matter
- The course supports material development for different applications based on colloidal systems.

Prerequisite:

- Basic knowledge of physical chemistry is helpful.
- Basic knowledge of colloids.
- Basic knowledge of Surfactants.

Unit-I Colloids and Interface: bridge to Nano science

Introduction, Interfaces, Interfacial properties, Electrical double layer, Colloids, Distinguish behaviour of colloidal particles, Interfacial Phenomena, The bridge to nanoscience, size dependent aspects of the colloidal nanoparticles, Nanostructures and assemblies, Buckyballs, Carbon nanotubes, Vesicles, Dendrimers, Nanoforests, Nanohelices, Nanoarrays, Generic nanoscience, New tools of generic nanoscience

Unit-II Surfactants based colloidal Nano Science

Structure of different types of surface active agents, Surfactant adsorption from aqueous solution, Uses of surface active agents, Classification of surfactants, Self-assembly of surfactant monomers in solution, Formation of micelles: critical micelle concentration (CMC) , Micellar solubilisation , Micellar shape and the Critical Packing Parameter.

Unit-IV Characterization of Nanoparticles

Introduction, Particle size distribution, Measurement techniques of particle size, Optical Microscopy, Electron Microscopy, Atomic Force Microscopy,Zonal methods, Electrical Sensing, Optical Sensing, Scattering Methods, Small-angle neutron scattering (SANS) and Small-angle X-ray scattering (SAXS), Analysis of scattered radiation, Characterization of the electrical properties of particles, Surface charge by titration.

Reference Books:

1. An Introduction to Interfaces & Colloids: The Bridge to Nanoscience by John C. Berg, World Scientific Publishing Co. Pte. Ltd., Singapore

2. Colloids and Interfaces with Surfactants and Polymers – An Introduction, by Jim W. Goodwin, John Wiley & Sons, Ltd,

3. Introduction to Colloid and Surface Chemistry by by Duncan J. Shaw, Butterworth-Heinemann

4. Principles of colloid and surface chemistry by Paul C. Hiemenz, Raj Rajagopalan, CRC Press; 3rd edition, 2016., Taylor & Francis, USA

5. Surface and Colloid Chemistry: Principles and Applications by K. S. Birdi, , CRC Press, Taylor & Francis, USA

Learning outcomes:

After completion the course, the learner shall be able to:

- Interpret the properties of colloidal systems by means of basic theories.
- Characterize colloidal system's properties.
- Critically evaluate literature in colloid and surface chemistry.

Dissertation (Credit 12)

(CH21250)