

O721 H Advanced Reaction Mechanism

Learning Objectives

The learning objectives of this course are to

- (i) Review the concepts of hard and soft acids and bases extending to ambient electrophiles and ambient nucleophiles.
- (ii) Impart detailed knowledge on Molecular Orbital (HMO) and Frontier Orbital (HOMO and LUMO) concepts and their applications to evaluate and interpret different reactions.
- (iii) Give knowledge on quantitative correlation of acidity and basicity of organic molecules and their effect on reaction rates, equilibria, substituents using different proposed equations such as Hammett equation, Yukawa-Tsuno equation etc.
- (iv) Impart knowledge on kinetics and reaction mechanism of substitution reaction, addition reaction, catalytic reaction and free radical reactions.
- (v) Give knowledge on the reaction mechanism of the medium and large ring compounds and non-benzoid aromatic compounds.

Course Content

1. **Modern Concepts of Acids and Bases, Nucleophiles and Electrophiles** incorporating orbital symmetry rules.
2. **Molecular Orbitals and Frontier Orbitals:** Hückel molecular orbital (HMO) method. Evaluation of aromaticity and the $4n+2$ rule in terms of HMO method. Prediction of thermal and/or photochemical reactions on the basis of aromatic and Möbius transition state concept. Calculation of resonance energy by using α (coulomb integral) and β (resonance integral). Frontier orbital theory; HOMO and LUMO; perturbation theory of reactivity; the α -effect; interpretation of ionic, pericyclic, sigmatropic and radical reactions in terms of frontier orbital theory.
3. **Quantitative Correlation of Acidity and Basicity:** Quantitative correlation of reaction rates and equilibria, general approach, correlation with *meta*-, and *para*-substituted benzene derivatives, correlation with relatively rigid non-aromatic compounds, deviation from Hammett equation. Quantitative correlation with acidity and basicity. Derivation of Hammett equation; Hammett's h_o function; Grunwald-Winstein acidity scale, polar effects in aliphatic compounds---Taft treatment. Linear Free Energy Relationship--- Hammett plots, Hammett equation, substitution constants (σ_x), reaction constant (ρ), significance of σ_x , and ρ . Calculation of k and K values, deviation from Hammett-straight-line plots. Yukawa-Tsuno equation, Taft equation, Grunwald-Winstein equation. Thermodynamic implications of all these equations, Recent Modification of Hammett equation.
4. **Kinetics and Energetics in Reaction Mechanism:** Consecutive reactions-the steady-state approximation; parallel reactions, reversible reactions, derivation of the rate expressions, variation in kinetics in acid and base-catalysed reactions; ambiguities in interpreting kinetic data; microscopic reversibility, correlation of reaction rates and equilibria.
5. **Substitution Reactions:** Comprehensive treatment of solvolytic reactions; substitution reactions of ambident nucleophiles; attempted correlation of substitution rates- the Swain-Grunwald equation; the Hammett equation and correlation with *meta*- and *para*-substituted benzene derivatives.
6. **Addition Reactions:** Multi-centre addition reactions- Diel's-Alder and *Retro* Diel's-Alder reactions, various types of dienes, and dienophiles, 1,3-dipolar additions, chelotropic reactions, and their stereochemistry. Nucleophilic addition to C=O group (the Cram's rule, stereochemical treatment) and related unsaturated system.

7. **Catalysis** : Acid-base catalysis, definitions and examples, mechanisms of acid and base-catalysed reactions, rate of acid and base-catalysed reactions. Classification of catalysts—electrophilic and nucleophilic catalysis, “physical” catalysis, acid-base catalysis, intramolecular catalysis, enzymic catalysis, catalysis of non-ionic reaction mechanisms.
8. **Molecular Rearrangement**: Carbocation rearrangements in bridged-bicyclic system—the norbornyl systems treating both classical and non-classical carbocations showing how anchimeric assistance plays its role. Rearrangements in small-ring compounds.
9. **Chemistry of Medium and Large-ring Compounds**: *Transannular* reactions.
10. **Chemistry of Non-Benzenoid Aromatic Compounds**: Azulenes and annulenes.
11. **Mechanism of Free Radical Reactions**:
Part I: Long-lived and short-lived free radicals - configuration of free radicals, generation and detection of free radicals, types of free radical reactions and some of their common characteristics.
Part II: Homolysis and free radical displacements - Iodine-exchange reactions, autoxidations, decomposition of various peroxides, azo and diazo compounds.
Part III - Additions and rearrangements of free radicals.
12. **Mechanistic aspects of ornamentations of organic compounds with multifunctionals taken from recent research review articles.**

Learning Outcome

Upon completion of this course, the students will be able to

- (i) Demonstrate the knowledge on hard and soft acids and bases extending to electrophiles and nucleophiles and their quantitative relationship.
- (ii) Understand the molecular orbital theory and orbital symmetry of organic molecules and appreciate both structural and chemical transformation of organic molecules.
- (iii) Understand the involved kinetics and energetic of reaction mechanism.
- (iv) Explain reaction mechanism of different types of reaction such as substitution, addition, catalytic, and free radical reactions.

Books Recommended

1. Mechanism in Organic Chemistry by Alder, Baker, and Brown (Wiley and Sons)
2. Frontier Orbital and Organic Reactions by Ian Fleming (Wiley and Sons)
3. Organic Reaction Mechanism by E S Gould (Holt, Rinehart, and Winston)
4. Organic Reaction Mechanism by Breslow (Benjamin Cummings and Co)
5. Organic Chemistry by Handrickson and Pine (McGraw Hill)
6. Physical Organic Chemistry by Neil S Isaac (Longman)
7. Physical Organic Chemistry by Jack Hine (McGraw Hill)

O 722 H Advanced Stereochemistry

Learning Objectives

The learning objectives of this course are to

- (i) Provide the fundamental concepts on symmetry, symmetry operations, symmetry and molecular properties, molecular dissymmetry etc.
- (ii) Gather knowledge on chiroptical properties, factors leading chirality. Application of different techniques and rule for the determination of structure, conformation and configuration.
- (iii) Have knowledge on stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- (iv) Impart knowledge on chirality in molecules devoid of chiral centres.
- (v) Convey knowledge on asymmetric synthesis.

Course Content

1. **Optical Activity:** Its origin, atomic and conformational asymmetry. Molecular symmetry and group theory Molecular dissymmetry.
2. **Variation of Optical Activity with Wavelength:** Optical rotatory dispersion and circular dichroism curves and their application in determining the configuration and conformation of different compounds.
3. **Conformational Analysis:** Reactivity of alicyclic, cyclic, fused and bridged ring systems, Curtin Hammet principle and its application in determining the course of reaction in different compounds.
4. **Tricovalent Carbon**
5. **Optical activity due to atoms other then carbon.**
6. **Optical isomerism due to restricted rotation:** Biphenyl isomerism, other examples of Atropisomerism (Binuclear compound, mononeuclear compound Ansa compound, Paracyclophane.
7. **Prostereoisomerism,Prochirality and Pseudochirality:** Terminology, homotopic and heterotopic ligands and faces, heterotopicity and nuclear magnetic resonance.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Demonstrate on chiroptical properties, factors leading to chirality, and apply different techniques and rules for the determination of structure, conformation and configuration.
- (ii) Understand stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- (iii) Find out chirality in molecules devoid of chiral centres and carry out asymmetric synthesis.

Books Recommended

1. Stereochemistry of Carbon Compounds: E.L.Eliel, McGraw Hill. New Delhi.
2. Stereochemistry of Organic Compounds: E.L. Eliel, Samuel. H., Wilen. John wiley & Sons.
3. Stereochemistry, Conformation and Mechanism: P.S. Kalsi, New Age International (P) Ltd., India
4. Stereochemistry of Carbon Compounds: G Hallas
5. Stereoselective Synthesis in Organic Chemistry Atta-ur-Rahman and Zahir Shah, Springer-Verlag.

O 723 H Spectroscopic Methods in Organic Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Review their knowledge about different types of spectroscopic technique i.e., UV, IR, NMR and MS.
- (ii) Impart knowledge on advanced techniques about one dimension and two dimension NMR studies.
- (iii) Understand advanced techniques about mass spectrometry and its application.
- (iv) Develop skill for analyses of UV-Visible, IR and NMR and Mass spectral data to elucidate the structure of organic compounds.

Course Content

- 1. UV, IR, Raman and ESR Spectra:** Review of the theory and experimental techniques, Application in the identification of organic molecules and free radicals.
- 2. NMR:** Theory, experimental methods, spin-spin couplings-AB system, ABX and ABX₂ systems etc. Internal rotation and the equivalence and non-equivalence of nuclei; variable temperature spectra, factors affecting coupling constants. Dynamic nuclear magnetic resonance and kinetic study of reactions. Chemically induced dynamic nuclear polarization, Relaxation effect, Spin-Lattice relaxation. Measurement of T₁ and T₂. Mechanism of spin-lattice relaxation, Application of Dipolar Relaxation Times, Spin-Spin Relaxation, The multiple Irradiation Techniques, Spectral simplification. Elimination of Quadrupolar effects. Multiple pulse sequence, Measurement of T₂, Spectral editing, Signal and resolution enhancement, Connectivity. Two dimensional NMR, COSY, NOESY, SECSY, EXTASY, INADEQUATE and RELAY experiments. COLOC experiments, HSQC, DEPT, HMBC, TOCSY & HETCOR experiments. Introduction to Tactics strategies of structure elucidation by one and two-dimensional NMR skeletal structure (atom connectivities) by NMR experiments. Relative configuration and conformation by NMR. ¹³C-NMR and theoretical calculation of ¹³C value. Applications of modern NMR techniques in the structure elucidation of organic compounds.
- 3. Mass Spectroscopy:** Theory, spectrometer and application to structure determination of organic molecules. Kinds of mass spectrum: Electron Impact (EI) & Chemical Ionization (CI), Fast Atom Bombardment (FAB), Secondary Ion Mass Spectroscopy (SIMS), Electron Spray (ES) & Thermo Spray (TS) spectra, Matrix Assisted Laser Ionization / Desorption (MALDI), Field Desorption (FD) & Plasma Desorption (PD). Tandem Mass Spectroscopy (MS-MS / MS-MS-MS). Analyzer: Magnetic Sector, Quadrupole, Ion Trap, Time-Of-Flight (TOF), Fourier Transform-ion Cyclotron Resonance (FTICR or FTMS). 3D-Mass spectroscopy. Circular dichroism (CD) and its application in configurational studies.
- 4. Following Progress of Reactions by Spectroscopy:** Diagnostic appearance and disappearance of functional groups in organic compounds and also in characterizing the products.
- 5. Structure Elucidation by Spectroscopy:** Combined application of UV, IR, NMR, and Mass spectroscopy in the structure elucidation of organic compounds- illustration with the spectra of typical compounds- Recognition of Structural Fragments by NMR, Introduction to Tactics and Strategies of Structural Elucidation by ONE and TWO Dimensional NMR.

6. Introduction to Recent Developed Spectroscopic Techniques taken from journals.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Identify compounds by analysis and interpretation spectral data.
- (ii) Analyze and interpret 1D and 2D NMR spectra.
- (iii) Learn how to use modern mass spectrometry techniques (CI, ESI, FAB, TOF, GC-MS, LC-MS/MS) to find out the molecular mass and structure.
- (iv) Acquire the ability to determine the structure of typical organic compounds using spectroscopic techniques.

Books Recommended:

1. Spectroscopic Identification of Organic Compounds: Bassier and Morril, John Willey and Sons.
2. Spectroscopic Methods in Organic Chemistry: D. H. Williams and I. Fleming, McGraw Hill, New-York
3. Spectroscopic Analysis: D. L. Pavia, G. M. Lampman and G. S. Kriz
4. Basic One- and Two-Dimensional NMR Spectroscopy: Horst Friebolin, WILEY-VCH, New-York
5. Mass Spectroscopy: H. C. Hill
6. Structure Elucidation by NMR in organic chemistry by Eberhard Breitmaier, University of Bonn, Germany.

O 724 H Chromatographic Techniques and Its Application in Analytical & Environmental Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on chromatography and its basic principle for separation, identification and quantification of organic compounds.
- (ii) Develop the knowledge to separate the mixture of components by TLC using different stationary phases.
- (iii) Impart knowledge on some advanced systems of chromatographic techniques such as DCCC, MLCCC, and SPE etc.
- (iv) Impart knowledge on gas chromatographic techniques with different columns and detectors and acquainted with their working principle.
- (v) Demonstrate advanced knowledge on HPLC with different detectors and their application for separation, identification and quantification of organic compounds.
- (vi) Provide the principle and applications of LC-MS.

Course Content

1. **Chromatographic Techniques:** Brief introduction of chromatography and its basic principles. Different kinds of stationary phases (normal, reversed, bonded phase etc.) for column, thin layer and size exclusion chromatography.
2. **High Performance Thin Layer Chromatography (HPTLC):** Principle and application of HPTLC. Different components of HPTLC; pre-coated plates, sample application device,

densometer, detector and recorder/integrator/computer. Identification and quantification of organic compounds by HPTLC.

3. **Gas Chromatography (GC) and GC-MS:** Gas chromatograph: gas chromatograph and its components. Types of Detector: Universal Detector & Specific detector. Thermal Conductivity Detector (TCD), Flame Ionization Detector (FID), Electron Captured Detector (ECD). Nitrogen Phosphorus Detector (NPD), Mass Detector (MSD), GC-IR & MS, GC with biological & Mass detectors. Cross sectional diagram, function, detection limit, linearity, sensitivity and specificity of each detector. Identification and quantification by GC. Head space GC and on-line head space GC & GC-MS. SIM and SCAN methods of GC-MS, use of NIST library, Method development and validation, Common trouble shooting in operating GC and GC-MS and routine maintenance, Quality Control and Quality Assurance (QC& QA).
4. **Liquid Chromatography:** An overview of LC and its components. . Different types of LC: Ultra performance liquid chromatography (UPLC) Capillary liquid chromatography (micro-HPLC), different types of detectors of LC: UV-VIS, Photodiode array, Fluorescence, Electrical conductivity, Refractive index, Light scattering mass and MS detectors, class of compounds to be separated by each detector. Advantages and limitations of each detector. UPLC; Size of column, particle size of stationary phase, pressure and temperature in separation compounds by UPLC. Chiral and ion exchange LC separations. Method development and method validation in LC operations. Use of LC-NMR in drug discovery. Common trouble-shooting in LC during operation and routine maintenance of LC.
5. **LC-MS and LC-MS-MS:** Introduction to LC-MS, different kinds of Ionization & Ionization Efficiency, mass analyzers Electro Spray Ionization (ESI), Atmospheric Pressure Chemical Ionization (APCI), Atmospheric Pressure Photo Ionization (APCI), Dual sources (ESI/APCI) or (APCI/APPI) system of ionization. Ionization Source Principles: Production of charged droplets, Evaporation, Droplet size reduction, and fission (Coulomb explosion), gas phase ionformation, clustering & declustering, curtain gas, corona charged needle etc. Mass Analyzer: Triple Quadrupoles (QQQ), Ion Trap (IT) and Hybrids. Effect of acids or bases in ionization process. Advantage of Ion Suppression in LC-MS. LC-MS-MS systems (Tandem mass): Tandem Mass Spectrometry Ion trap (traditional special traps), Triple quadruple (QQQ), and QTrap systems. Modes of MS-MS analysis Specificity and sensitivity of LC-MS and LC-MS-MS; Common trouble shooting in operating LC, LC-MS and LC-MS-MS. Requirements for getting accreditation of analytical laboratory.

Learning Outcomes

Upon completion of this course, the student will be able to

- (i) Understand the basic principles of various chromatographic techniques and demonstrate different related terms.
- (ii) Acquainted with the principles and application of paper, thin layer and ion-pair chromatographic techniques.
- (iii) Apply chromatographic techniques such as HPLC, GC and GC-MS for the separation, identification, and quantification of organic molecules using different detectors.
- (iv) Demonstrate and apply knowledge on analyzing various types of samples using LC-MS.
- (v) Review and compare some advanced chromatographic techniques for their application in different organic samples.

Books Recommended:

1. Practical Liquid Chromatography: S. G. Perry, R. Amos and P. I. Brewer, Plenum Press, New York /, London.
2. Analytical Chemistry Principles: John. H. Kennedy, Second Edition, Saunders College Publishing, New York
3. Chemical Analysis: H. A. Laitinen.
4. Fundamentals of Analytical Chemistry: D. Skoog, D. M. West and F. G. Holler, Fifth Edition, Sanders College Publishing, New York
5. High Performance Liquid Chromatograph: Sandy Lindsay, John Wiley & Sons
6. Instrumental Methods of Chemical Analysis: Glen. W. Ewing
7. Modern Methods of Chemical Analysis: Pecsok and Shields
8. Analytical Chemistry: Gray. D. Christian, 5th Edition, John Wiley & Sons
9. Practical HPLC: Veronica, R. Meyer, 2nd Edition, John Wiley & Sons
10. HPLC, A practical guide: T. Hanai, RAC 1999
11. Analytical Chemistry Handbook: John A Dean, McGraw Hill

O 725 H Organic Syntheses**Learning Objectives**

The learning objectives of this course are to

- (i) Provide basic concepts on the strategy for carrying out an organic synthesis process.
- (ii) Impart knowledge for developing ability to plan and carry out synthetic experiments independently.
- (iii) Grow critical awareness of advances at the forefront of new methodologies in the synthesis of biologically important organic molecules.

Course Content

1. **Synthesis and Retrosynthesis:** Routine for designing a synthesis, technical terms for the disconnection approach, strategy and guidelines to good disconnections.
2. **The Disconnection approach:** One group C-X disconnection. One group C-C disconnection: alcohols and carbonyl compounds. Two group disconnection: 1,5-Difunctionalized compounds, Michael addition and Robinson Annulation.
3. **Selective reactions and protection:** Application of protecting groups in protection of aldehydes, ketones and alcohols. The protecting groups are Acetal (dioxolane), trialkylsilyl (TBDMS), tetrahydropyranyl (THP) and benzyl ether (OBn). Synthesis of oxitocin, gastrin and aspartame (using protecting groups).
4. **Reaction Intermediates in organic synthesis with particular reference to:** Carbenes, ketenes and nitrene (electronic structure and energy, generation reaction type chemical activation, structure and reactivity). Enamines and heterocyclic enamines (Preparation and Reactions).

5. **Organometallic Reagents in organic synthesis:** The principles, reactions of organometallic compounds, Grignard reagents, organocopper reagents, using organometallic reagents to make C-C bonds, Heck reactions, Suzuki reactions.
6. **Oxidation and Reduction methods in synthesis:** Catalytic hydrogenation, dissolving metal reduction, metal hydride reduction and related reactions, oxidation with chromium and manganese compounds, peracids and peroxides, mercuric acetates and selenium dioxide.
7. **Stereoselective synthesis:** Regioselective, diastereoselective, enantioselective and chemoselective synthesis. Synthesis of chiral compounds.
8. **Design of Drug synthesis:** Structure activity relationship, use of retrosynthesis in designing synthesis of biologically important organic compounds. Synthesis of some typical medicinal compounds- Ascorbic acid, β -carotene, prostaglandins ($F_{2\alpha}$ and E_2), taxol, oestrone and salbutamol.
9. **Combinatorial synthesis:** Principles, illustration with selected examples, advantages and limitations of combinatorial synthesis.

Learning Outcomes

After completing the course, the students should be able to

- (i) Carry out different synthesis and transformation of the most common functional groups.
- (ii) Describe and apply stereochemical concepts such as chirality, stereoisomerism, and stereoselectivity in relation to chemical transformations.
- (iii) Identify, analyze and evaluate synthetic routes to target molecules by one-group and two group disconnections.
- (iv) Apply organometallic reagents and reactions in organic synthesis.
- (v) Plan and design experimental setups for various types of synthesis of biologically important organic compounds.

Books Recommended:

1. Stereoselective Synthesis in Organic Chemistry: Atta-ur-Rahman & Zahir Shah, Springer Verlag
2. Principles of Organic Synthesis: Norman, Methuen & Co. Ltd
3. Modern Synthetic Reactions: H. O. House
4. Advanced Organic Chemistry: Reaction Mechanism and Structure: Jerry March
5. Fundamentals of organic reaction mechanisms. J. Milton Harris and Carl C. Wamser
6. Reactive Molecules: Curt Wentrup
7. The disconnection approach : Wiley and Warren, S.
8. Advances in Heterocyclic chemistry : S. F. Dyke
9. Organic chemistry: Clayden, Greeves, Warren and Wothers.

O 726 H: Chemistry of Advanced Carbohydrates and Glycoconjugates.

Learning Objectives

The learning objectives of this course are to

- (i) Give advanced knowledge on monosaccharides and their different structural features in different situations.
- (ii) Impart knowledge on synthesis of glycosides, anhydro-, amino-, and deoxy-sugars and their reactions.
- (iii) Have knowledge on the importance of polysaccharides and their industrial and biological importance.
- (iv) Acquire knowledge for isolation, purification and structural elucidation of complex polysaccharides.
- (v) Review the important polysaccharide derivatives and their applications.

Course Content

1. Review of chemistry of structure, configuration and conformation of monosaccharides. Properties of carbohydrates in relation to their shapes and conformation. Stability and anomeric ratio of pyranoses and furanoses.
2. Different reactions of monosaccharides at anomeric and non-anomeric carbon atoms. Synthesis and reactions of glycosides, amino sugars, anhydro sugars, deoxy sugars, thio sugars and halo sugars. Uses of different blocking and deblocking agents in different reactions of carbohydrates moiety. Synthesis of Uronic acids and complex carbohydrate derivatives (i.e, Streptose, ATP, ADP)
3. Chemistry of polysaccharides of different sources: Plants, Microorganism, Algae and Seaweeds. Classification, isolation and purification of polysaccharides, Physical (including spectroscopic) and chemical methods of structure elucidation of polysaccharides. Different physical and chemical methods of determination of molecular weight and D. P. of carbohydrate polymer.
4. General structure of macromolecular carbohydrates (Primary, secondary and tertiary structure)
5. Chemistry of dietary fiber: Sources, classification, methods of isolation, purification and linkage pattern of different dietary fiber. Importance of dietary fiber in prevention of different diseases.
6. Chemistry of glycoconjugates: Sources, structure and biological importance of glycoprotein, proteoglycan, different glycolipids and glycosaminoglycans.
7. Different derivatives of polysaccharides and their technological aspects of applications.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the monosaccharide chemistry.
- (ii) Find out route to synthesize different monosaccharide derivatives.
- (iii) Understand the techniques of isolation and purification of complex polysaccharides..
- (iv) Elucidate the structure of complex polysaccharides using chemicals and spectroscopic means
- (v) Prepare industrially and biologically important polysaccharides derivatives and use them for suitable purposes.

Books Recommended

1. Advanced in Carbohydrate Chemistry (Series).

2. Methods in Carbohydrates (Series).
3. Monosaccharides - Their Chemistry and Their Roles in Natural Products, P. M. Collins and R. J. Ferrier.
4. Polysaccharides, Vol. I-V, G. O. Aspinall.
5. Principles of Biochemistry, A. L. Lehninger.

O 727 H Natural Products

Learning Objectives

The learning objectives of this course are to

- (i) Give basic knowledge on extraction, isolation & purification of natural products.
- (ii) Develop clear understanding of the chemistry of important natural products like terpenoids, alkaloids, steroids, hormones and natural pigments.
- (iii) Know the structural features of polymers like polysaccharides, proteins and nucleic acids.
- (iv) Develop knowledge on biosynthesis of natural products.
- (v) Have basic idea about natural products from marine sources

Course Content

1. **Chemistry of Living Species:** Anabolism and catabolism through metabolism in nature. The role of biogenetic groupings in chemotaxonomic classification of plants.
2. **Different Pathways of Biosynthesis of:** Secondary metabolites such as acetate fatty acid, polyketides-mevalonates, isoprenoids, shikimic acid and amino acids.
3. **Importance of Secondary Metabolites and Plant Ecology in Nature:** Plant-herbivore interaction, plant-insect interaction, plant-plant interaction and plant microorganism interaction.
4. **Application of Chemical, Spectroscopic and Chromatographic Methods:** In phytochemical studies.
5. **Chemical Characterization and Structural Elucidation of Natural Plant Materials:** Isolation, separation, purification and identification of their physiological actions by degradative and spectroscopic methods occurring in plants with an emphasis on terpenoids, steroids, carotenoids, alkaloids, vitamins and natural pigments with reference to citral, zenziberine, ergosterol, testosterone, β caroteine, morphine, ratinols, indigotin, flavones, haemoglobin and their biological activity.
6. **Chemical Characterization and Structural Elucidation of Natural Polymer** with an emphasis on of polysaccharides, proteins, wool and nucleic acids. Composition and biological function of insulin, glycoprotein, lipoprotein and nucleoprotein etc.
7. **Lipids:** Important physical as well as chemical characterization and classification of nonsaponifiable lipids and the biological function of glycolipids, phospholipids VLDL, LDL and HDL and their characteristics chemical properties.
8. **Pheromones:** Chemistry of pheromones, their importance and function in biological systems.

Learning Outcomes

Upon completion of this course students will be able to

- (i) Apply the extraction, isolation and purification techniques of different natural products like terpenoids and alkaloids.

- (ii) Demonstrate the steps of biosynthesis of carbohydrates, terpenoids alkaloids and steroids.
- (iii) Characterize different polysaccharides, proteins, terpenoids, carotene flavonoids and alkaloids by chemical as well as spectroscopic methods.
- (iv) Explain the functions of natural products and polymers like natural pigments, carotenoids, flavonoids etc.
- (v) Discuss the chemistry of different types of steroids, hormones steroidal alkaloids.

Books Recommended

1. Organic Chemistry, Vol. 2: Stereochemistry and Chemistry of Natural Products: I. L. Finer.
2. Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis: J. B. Harborne.
3. Secondary metabolites: J Mann (Clarendon Press, Oxford 1987).
4. Chemistry of organic Natural Products; Agarwal, Vol. I & II; Geol Publishing House. UP. India.
5. Trease and Evans Pharmacognosy — W.C. Evans, 15th edn. Saunders, Edinburgh.
6. Organic Chemistry, Francis A. Carey, 3rd edn. The McGraw-Hill Companies, Inc; ISBN-0-07-114092-1

O 728 H Advanced Heterocyclic Compounds and Caged Hydrocarbons

Learning Objectives

The learning objectives of this course are to

- (i) Give the advanced understanding of heterocyclic chemistry.
- (ii) Acquaint with the idea about structure, properties, synthesis and reactions of the important heterocyclic compounds, as well as different systems of nomenclature.
- (iii) Impart advanced knowledge on the designing of synthetic routes for different heterocyclic compounds.
- (iv) Develop knowledge about preparation, properties and applications of caged hydrocarbons.

Course Content

1. **Introduction:** Importance and applications of heterocyclic compounds; Classification; Systematic nomenclature for monocyclic, fused and bridged heterocycles.
2. **Five-Membered Heterocycles with Two Heteroatoms:** Synthesis, physico-chemical properties and uses of nitrogen-nitrogen (pyrazoles, imidazoles and related compounds), nitrogen-oxygen (oxazoles, isooxazoles and related compounds), nitrogen-sulphur (thiazoles, isothiazoles and related compounds).
3. **Benzo-fused five-membered heterocycles with one heteroatom:** Synthesis and reactions of benzopyrroles, benzofurans, and benzothiophenes.
4. **Benzo-fused five-membered heterocycles with two heteroatoms:** Synthesis and physico-chemical properties of benzimidazoles, indazoles, benzoxazoles, benzthiazoles and related compounds.

5. **Six-membered heterocycles with one heteroatom:** Synthesis and reactions of pyridine derivatives (Alkyl and aryl pyridines, aminopyridines, halopyridines, hydroxypyridines, pyridine N-oxides, pyridine aldehydes and ketones, pyridinium salts), quinolines, isoquinolines, acridines and phenanthridines. Synthesis and reactions of pyrylium salts, pyrones, benzopyrylium salts, coumarins and chromones.
6. **Six-membered heterocycles with two or more heteroatoms:** Synthesis and reactions of diazines, triazines, tetrazines and thiazines.
7. **Seven and large membered heterocycles:** Synthesis and reactions of azepines, oxepines, thiepinines, diazepines, thiazepines, diazocines, dioxocines and dithiocines.
8. **Meso-ionic heterocycles:** General classification, chemistry, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.
9. **Selenaheterocyclic compounds of practical importance.**
10. **Adamantane and related polycyclic systems.**
11. **Fullerenes.**

Learning Outcomes

Upon completion of this course, the student will be able to

- (i) Understand the importance of heterocyclic compounds in biological systems, pharmaceuticals and other industrial applications.
- (ii) Plan synthetic route of major classes of heterocyclic compounds.
- (iii) Demonstrate mechanisms for reactions involving heterocycles as starting materials, intermediates and products.
- (iv) Understand the preparation, properties and applications of caged hydrocarbons.

Books Recommended

1. E. H. Rodd, Chemistry of Carbon Compound (Heterocyclic Compounds), IV A,B,C.
A. R. Katritzky, Advances in Heterocyclic Chemistry.
2. G. M. Badger, The Chemistry of Heterocyclic Compounds.
3. J. A. Joule, K. Mills and G. F. Smith, Heterocyclic Chemistry.
4. M. Lagowski and A. R. Katritzky, The Principles of Heterocyclic Chemistry.
5. R. K. Bansal, Heterocyclic Chemistry.
6. R. M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds.
7. T. L. Gilchrist, Heterocyclic Chemistry.
8. R. O. C. Norman, Principles of Organic Synthesis.
9. T. Eicher, S. Hauptmann and A. Speicher, The Chemistry of Heterocycles.
10. R. R. Gupta, M. Kumar and V. Gupta, Heterocyclic Chemistry

O 729 H Organic Pollutants in the Environment

Learning Objectives

The learning objectives of this course are to

- (i) Introduce general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Give general concept on toxicants and their doses, accumulation in organism and excretion.
- (iii) Impart knowledge on pollution by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, fertilizers and their management.
- (iv) Acquaint with the pollution by traditional and modern pesticides, plant growth regulator and their formulation and various actions also food safety and poisoning.
- (v) Gain concepts on integrated pest management to reduce pollution.

Course Content

- 1. Organic pollutants, their sources and behavior in the Environment:** Brief description about organic pollutants in the atmosphere, their persistence, Bioaccumulation, Biomagnification, Biodegradation and Biotransformation. Persistent Organic Pollutants (POPs) and their effects on human and wild animals. Biogenic organic compounds.
- 2. Environmental Toxicology:** Introduction to toxicology & ecotoxicology. Dose-response relationship. Dose & frequency of use. Routes and mechanism of entry of toxicants to organism, Distribution of toxicants within the organism and biotransformation, excretion; Classes of poisons based on Effect, Quantitative principles of Toxicology.
- 3. Pollution by Hydrocarbons and related compounds:** Occurrence, Chemical nature; Dispersion, Evaporation, photooxidation & microbial transformation in the environment and aquatic organisms of Petroleum, polycyclic aromatic hydrocarbons (PAHs), Polychlorinated Biphenyls (PCBs), Hydroxylated PCBs (OH-PCBs), and Dioxins. Environmental distribution, Persistency, Toxicity, Carcinogenicity of these compounds to human and wild life.
- 4. Industrial pollutants and their management:** Pollutants from Industries with special references to Polymers & Plastic, Soap & Detergents, Pulp & Paper, Chemical & Pharmaceutical industries. Abatement procedures for the reduction of pollution from different industries.
- 5. Organic pollutants from agriculture:** Pesticides (Insecticides, Herbicides & Fungicides): Classification, uses and effects on environment and human health with reference to Traditional and Modern pesticides. Mechanism of action and metabolism of pesticides in biological system. Detoxification and their metabolites in the environment. **Traditional Pesticides:** Organochlorine (DDT, Heptachlor, Endosulfan, HCH, HCB), Organobromine and Organofluorine compounds. **Modern Pesticides:** Organophosphorous and organothiophosphorous (Diazinon, Malathion, Chlorpyrifos, Parathion, Parathion-methyl), Carbamic Acid Derivatives (Carbaryl, Pirimicarb, etc.) Phenoxy Acid Derivatives (2,4-D MCPA, MCPB, etc). MRL values and ADI of some common pesticides recommended by Codex Alimentarius Commission, United States Food and Drug Administration (USFDA) and World Health Organization (WHO). **Formulation of pesticides:** Wettable powder, emulsion/solution and fumigants, etc. Insect attractant, repellent and chemosterile retardants. Plant growth regulators.
- 6. Fertilizers.**

7. **Pollutants in Food:** Safe food, Chemical contaminants in food: aflatoxin, isoflavones, sinigrin, heavy metals, etc. **Artificial contaminants in food:** Synthetic food colors, dyes and pigments, etc. **Harmful Antibiotics in Food:** Nitrofurans and its metabolites, chloramfenicol, etc.
8. **Pollution of Environment by hazardous waste materials:** Nature, Sources and environmental Chemistry of hazardous wastes, Hazardous wastes in atmosphere hydrosphere and biosphere, microbial metabolism in waste degradation, Safe disposal by proper chemical & biological treatment of city waste, domestic & hospital wastes.
9. **The role of integrated pest management to control pollution:** Integrated pest Management (IPM): Definition, Key components of IPM, Pest control techniques, Reduction of pollution. IPM in context of Bangladesh. Biopesticides and use of biopesticides to produce organic agricultural products. Pest control by Pheromones. Use of pheromones in context of Bangladesh agriculture.

Learning Outcomes

Upon completion of the course, the students will be able to

- (i) Demonstrate general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Apply general concept on toxicants and their doses.
- (iii) Manage various pollutions by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, and fertilizers.
- (iv) Assess pollution by traditional and modern pesticides, their formulation also food poisoning and its safety.
- (v) Suggest integrated pest management plan to reduce pollution.

Books Recommended

1. Basic Concept of Environmental Chemistry: Des. W. Connell. Lewis Publishers
2. Fundamental Concept of Environmental Chemistry, G. S. Sodhi. Narosa Publishing House.
3. Organic Chemicals: An Environmental Perspective, Alasdair, H. Neilson, Lewis Publishers.
4. Environmental Chemistry, A. K. Dey.
5. Environmental Pollution Analysis, Khopkar, Willey Eastern Ltd.
6. Environmental Chemistry: Stoker & Seager.
7. Environmental Chemistry (8th Ed.): Stanley E. Manahan, CRC Press, New York, 2005.
8. Handbook of Environmental Chemistry Series: Ed. O. Hutginger
9. Environmental Toxicology: M. Stake, M. Mida, M. S. Sethi. S. A. Iqbal, H. Yasuhisa and Taguchi, Discovery Press 2001.

O 730 H Advanced Medicinal Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Give general aspects of the design & development of drugs including their classification, methods and routes of administration and production.
- (ii) Impart knowledge on structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR), correlation of physicochemical properties, affection drug action and pharmacokinetics.
- (iii) Explain drugs action on nucleic acids, enzyme and proteins.
- (iv) Have knowledge on combinatorial synthesis for drug optimization and discovery.
- (v) Understand immunity, immunoglobulin, allergy, antihistaminic agents, cancer and anticancer agents.

- 1. Introduction:** Definition and classification of drugs, drug discovery and design, relationship between molecular structure and biological activity, physiological properties of drugs, stereochemistry and drug action.
- 2. Quantitative Structure-activity Relationships (QSAR):** Structure-activity relationship (SAR), Quantitative structure activity relationship (QSAR), introduction, physiochemical properties, Hansch equation, Craig plot, bioisosteres, and molecular modeling, computer aided drug design.
- 3. Combinatorial Synthesis for Drugs:** Principle of combinatorial synthesis, combinatorial synthesis for drug optimization and discovery, combinatorial synthesis in solid phase and solution phase. high- throughput screening (HTS).
- 4. Receptors and Drug Action:** Introduction to receptors and messengers, receptor binding and drug discovery, drug receptors and the biological response, receptor subtypes, neurotransmitters, neurotransmission processes, agonist and antagonist, design of agonists and antagonists, partial agonists.
- 5. Drugs Acting on Nucleic Acids:** Antimetabolites, enzyme inhibitors, intercalating agents, alkylating agents, antisense drugs, and chain-cleaving agents.
- 6. Immunobiologicals:** Cells of the immune system, immunity, innate immunity and acquired immunity, acquisition of immunity, immunoglobulins, antigen-antibody reactions and vaccine.
- 7. Histamine and Antihistaminic Agents:** Histamine, histamine life cycle, biosynthesis and distribution, storage and release of histamine, inhibition of histamine release, anti-histaminic agents, first generation and second generation antihistamine, allergens.
- 8. Cancer and Cancer Chemotherapy:** Introduction, definition, biochemical bases and causes of cancer, type of cancers, cancer therapy, class of anticancer agents and their mechanism of actions.

9. Medicinal Chemistry of Herbs: Herb, herbal purity and standardization, herb as a drug, types of herbs, chemistry and pharmacological activity of some herbs (*Capsicum*, *Garlic*, *Ginkgo biloba*, *Ginseng*, *Catharanthus roseus*).

Learning Outcome

Upon completion of the course, the students will be able to

- (i) Understand importance of chemistry in the development and application of therapeutic drugs.
- (ii) Relate the structure and physical properties of drugs to their pharmacological activity.
- (iii) Understand the physico-chemical properties of drugs, the present drug development process and design new drug with the help of new scientific techniques.
- (iv) Understand how changes in the chemical structure of drugs affect efficacy.
- (v) Describe the overall process of drug discovery, and the role played by medicinal chemistry in this process.

Books Recommended:

1. Foye's Principles of Medicinal Chemistry, 5th edn, David A Williams and Thomas L. Lemke, Lippincott Williams & Wilkins, Philadelphia, 2002.
2. An introduction to Medicinal Chemistry, 2nd edn, Graham L. Patrick, Oxford University Press, Oxford, 2001.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 11th edn, John H. Block and John M. Beale, Jr., Lippincott Williams & Wilkins, Philadelphia, 2004.
4. Medicinal Chemistry: An Introduction, Gareth Thomas, John Wiley & Sons, Ltd, Chichester, 2000.
5. Burger's Medicinal Chemistry and Drug Discovery, 5th edn, edited by Manfred E. Wolff, A Wiley-Interscience Publication, New York, 1995.
6. Bentley and Driver's Textbook of Pharmaceutical Chemistry — L.M. Atherden, 17th edn, Oxford University Press, London.
7. Pharmacognosy — V.E. Tyler, L. R. Brady & J.E. Robbers, 9th edn. , Lea & Febiger, Philadelphia.
8. British Pharmacopoeia Vol.I & II (latest edn.)

O 731 H Food Chemistry & Technology

Learning Objectives

The learning objectives of this course are to

- (i) Acquire knowledge about nutritional value, taste, texture and freshness of food and food products.
- (ii) Understand food constituent and their interactions under different conditions.
- (iii) Find the methods to preserve and enhance availability and quality of food.
- (iv) Impart integral knowledge on the food science and technology.

Course Content

1. **General Introduction:** Food, macro- and micro-nutrients in food. Digestion, absorption, metabolism.
2. **Carbohydrate:** Source of different types of starch and their consumption. Glycemic index of starch. Dietary fiber (DF), importance of high and low DF content in staple food. Addition of DF in bakery and other food products. Cereals and their uses.
3. **Chemistry of Protein Occurs in:** Fish, meat, eggs, milk & milk products, lentils etc and their nutritional values.
4. **Chemistry of Lipids:** Source, edible and non-edible fats/oils, their occurrence and consumption in food items. Free fatty acid, ω -fatty acids, *trans*-fatty acids and their effects on human health.
5. **Sugars:** Plant sugar and artificial sweeteners (saccharine, cyclamate, sucroluse, sorbitol, aspartame, di-peptide etc.) in food items.
6. **Food Additives:** Natural coloring agents, synthetic flavoring and coloring agents, and preservatives in food stuff, carotenoids, tocopheroles, flavonoids and anthocyanenes, vitamins and minerals.
7. **Toxicants:** Naturally occurring chemical toxicants (anthocyanines, safrole etc.) in foods and other food stuff, other contaminants in food stuff (pesticide residues and heavy metal).
8. **Genetically Modified Food:** Introduction, importance in food safety and security and their future prospect.
9. **Processed Food:** Process of bakery, milk products and juices, preservations and their nutritional values.

Learning Outcomes

Upon completion of the course, the students will be able to

- (i) Have general knowledge on food chemistry, such as carbohydrate, protein, lipids, etc.
- (ii) Gain in-depth knowledge on food additives, adulteration and food toxicants.
- (iii) Understand the general idea of genetically modified food and its future prospect.
- (iv) Understand modern food processing and preserving technology.

Books Recommended:

1. Food Chemistry, L. H. Meyer, Reinhold Publishing Corporation, New York.
2. Chemistry of Food and Nutrition, H. C. Sherman, The Macmillan Company, New York.

3. Advanced Text Book on Food and Nutrition, Vol I and II, 2nd edn., M. Swaminathan, Bappco, India.
4. Introductory Foods, 16th edn., M. Bennion, Merrill Prentice Hall, N.J.
5. Food Science and Nutritional Health: An Introduction. T. P. Labuza and J.W. Erdman, Jr., West Publishing Co.
6. Food Science, 2nd edn., H. Charley, John Wiley & Sons. Inc. New York
7. Foods and Food Production Encyclopedia, D.M. Considine and G.D. Considine, Van Nostrand Reinhold Co.

OC 601 H Advanced Organic Reaction Mechanism

Learning Objectives

The learning objectives of this course are to

- (i) Review the concepts of hard and soft acids and bases extending to ambient electrophiles and ambient nucleophiles.
- (ii) Impart detailed knowledge on Molecular Orbital (HMO) and Frontier Orbital (HOMO and LUMO) concepts and their applications to evaluate and interpret different reactions.
- (iii) Give knowledge on quantitative correlation of acidity and basicity of organic molecules and their effect on reaction rates, equilibria, substituents using different proposed equations such as Hammett equation, Yukawa-Tsuno equation etc.
- (iv) Impart knowledge on kinetics and reaction mechanism of substitution reaction, addition reaction, catalytic reaction and free radical reactions.
- (v) Give knowledge on the reaction mechanism of the medium and large ring compounds and non-benzoid aromatic compounds.

Course Contents

1. **Molecular orbitals and frontier orbitals:** Hückel molecular orbital (HMO) method. Evaluation of aromaticity and the $4n+2$ rule in terms of HOMO method. Prediction of thermal and/or photochemical reactions on the basis of aromatic and Möbius transition state concept. Calculation of resonance energy by using α (Coulomb integral) and β (resonance integral). Frontier orbital theory: HOMO and LUMO; perturbation theory of reactivity: the α -effect; interpretation of ionic, pericyclic, and radical reactions (substitution and addition reactions) in terms of frontier orbital theory.
2. **Acids and Bases, Nucleophiles and Electrophiles:** Classification on the basis of structures of organic molecules; hard and soft acid and bases (HSAB) based on HOMO theory; hard and soft nucleophiles and electrophiles; ambident nucleophiles.
3. **Quantitative Correlation of acidity and basicity:** Derivation of Hammett H_o function; Grunwald-Winstein acidity scale, polar effects in aliphatic compounds---Taft treatment.
4. **Kinetics and energetics in reaction mechanism:** Consecutive reactions-the steady-state approximation; parallel reactions, variation in kinetics in acid and base-catalysed reactions; ambiguities in interpreting kinetic data; microscopic reversibility, correlation of reaction rates and equilibria.
5. **Substitution reactions:** Comprehensive treatment of solvolytic reactions; attempted correlation of substitution rates- the Swain-Grunwald equation; the Hammett equation and correlation with *meta*- and *para*-substituted benzene derivatives.
6. **Addition reactions:** Multi-centre addition reactions; Carbonyl addition-Cram's rule (stereochemical concept) Nucleophilic addition to related unsaturated system.
7. **Molecular rearrangement:** Carbonium ion rearrangements in bridged-bicyclic systems particularly norbornyl system treating both classical and non-classical carbonium ions showing how anchimeric assistance plays its role. Rearrangements in small-ring compounds.
8. **Mechanism of free radical reactions.**

Learning Outcome

Upon completion of this course, the students will be able to

- (i) Demonstrate the knowledge on hard and soft acids and bases extending to electrophiles and nucleophiles and their quantitative relationship.
- (ii) Understand the molecular orbital theory and orbital symmetry of organic molecules and appreciate both structural and chemical transformation of organic molecules.
- (iii) Understand the involved kinetics and energetic of reaction mechanism.
- (iv) Explain reaction mechanism of different types of reaction such as substitution, addition, catalytic, and free radical reactions.

Books Recommended

1. Mechanism in Organic Chemistry by Alder, Baker, and Brown (Wiley and Sons).
2. Frontier Orbital and Organic
3. S Gould (Holt, Rinehart, and Winston).
4. Organic Reaction Mechanism by Reactions by Ian Fleming (Wiley and Sons).
5. Organic Reaction Mechanism by E Breslow (Benjamin Cummings and Co).
6. Organic Chemistry by Handrickson and Pine (McGraw Hill).
7. Physical Organic Chemistry by Neil S Isaac (Longman).
8. Physical Organic Chemistry by Jack Hine (McGraw Hill)

OC 602 H Advanced Stereochemistry

Learning Objectives

The learning objectives of this course are to

- (i) Provide the fundamental concepts on symmetry, symmetry operations, symmetry and molecular properties, molecular dissymmetry etc.
- (ii) Impart knowledge on chiroptical properties, factors leading chirality. Application of different techniques and rule for the determination of structure, conformation and configuration.
- (iii) Have knowledge on stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- (iv) Impart knowledge on chirality in molecules devoid of chiral centres.
- (v) Convey knowledge on asymmetric synthesis.

Course Content

1. **Optical Rotation and Rotatory Power (Chiroptical Properties):** Factors leading to chirality-. Elements of symmetry, Molecular symmetry and group theory. Molecular dissymmetry. Atomic asymmetry and conformational asymmetry. *Circular birefringence* and circular dichroism (CD). Optical rotatory dispersion (*ORD*). *Cotton effect*. Description of *ORD* curve. *Haloketone rule* and *Octant rule*. Application of these in determining the structure, conformation and configuration of different compounds.
2. **Conformational Analysis:** Conformation and reactivity in alicyclic, cyclic (medium and large size rings) fused and bridged ring systems (heterocyclics, decalins, anthracenes,

phenanthrenes, paddlances and propellanes, catenanes, rotaxane, knot, mobius strip, cubane, tetrahedrane, dodecahedrane, adamantane and buckminsterfullerene). *Curtin Hammett principle*, its application in determining the course of reaction.

- 3. Stereochemistry of Tricovalent Carbons:** Carbonium ions and carbanions.
- 4. Optical Activity due to Atoms other than Carbon:** Nitrogen, phosphorus, arsenic, sulphur, selenium.
- 5. Prostereoisomerism, Prochirality and Pseudochirality:** Terminology, homotopic and heterotopic ligands and faces, heterotopicity and nuclear magnetic resonance.
- 6. Atropisomerism:** Nomenclature, synthesis and stereochemistry of biphenyls, allenes and spiranes, molecular propellers and gears, helicenes, molecules with planar chirality.
- 7. Asymmetric Synthesis:** Introduction, diastereoselective synthesis, *Cram's rule*, enantioselective synthesis, double stereodifferentiation.

Learning Outcomes

Upon completion of this course, the students will be able to

- Demonstrate on chiroptical properties, factors leading to chirality, and apply different techniques and rules for the determination of structure, conformation and configuration.
- Understand stereochemistry of trivalent carbon, optical activity due to atoms other than carbon, prostereoisomerism, prochirality and pseudochirality.
- Find out chirality in molecules devoid of chiral centres and carry out asymmetric synthesis.

Books Recommended

- Stereochemistry of Carbon Compounds: E.L.Eliel, McGraw Hill. New Delhi.
- Stereochemistry of Organic Compounds: E.L. Eliel, Samuel. H., Wilen. John wiley & Sons.
- Stereochemistry, Conformation and Mechanism: P.S. Kalsi, New Age International (P) Ltd., India
- Stereochemistry of Carbon Compounds: G Hallas
- Stereoselective Synthesis in Organic Chemistry Atta-ur-Rahman and Zahir Shah, Springer Verlag.

OC 603 H Spectroscopic Methods in Organic Chemistry

Learning Objectives

The learning objectives of this course are to

- Review their knowledge about different types of spectroscopic technique i.e., UV, IR, NMR and MS.
- Impart knowledge on advanced techniques about one dimension and two dimension NMR studies.
- Understand advanced techniques about mass spectrometry and its application.
- Develop skill for analyses of UV-Visible, IR and NMR and Mass spectral data to elucidate the structure of organic compounds.

Course Content

- UV, IR, Raman and ESR spectra:** Review of theory and experimental techniques, Application in the identification of organic molecules and free radicals.
- NMR:** Theory, experimental methods, spin-spin couplings-AB system, ABX and ABX₂ systems etc. Internal rotation and the equivalence and non-equivalence of nuclei, variable

temperature spectra, factors affecting coupling constants. Dynamic nuclear magnetic resonance. Chemically induced dynamic nuclear polarization, Relaxation effect, Spin-Lattice relaxation. Measurement of T₁. Mechanism of spin-lattice relaxation, Application of Dipolar Relaxation Times, Spin-Spin Relaxation, ¹³C-NMR and theoretical calculation of ¹³C value. Applications of modern NMR techniques in the structure elucidation of organic compounds.

- 3. The multiple Irradiation Techniques:** Spectral simplification. Elimination of Quadrupolar effects. Multiple pulse sequence, Measurement of T₂, Spectral editing, Signal and resolution enhancement, Connectivity. Two dimensional NMR, COSY, NOESY, SECSY, EXTASY, INADEQUATE and RELAY experiments. COLOC experiments, HSQC, DEPT, HMBC, TOCSY & HETCOR experiments. Introduction to Tactics strategies of structure elucidation by one and two-dimensional NMR skeletal structure (atom connectivities) by NMR experiments. Relative configuration and conformation by NMR.
- 4. Mass spectroscopy:** Theory, spectrometer and application to structure determination of organic molecules. Kinds of mass spectrum: Electron Impact (EI) & Chemical Ionization (CI), Fast Atom Bombardment (FAB), Secondary Ion Mass Spectroscopy (SIMS), Electron Spray (ES) & Thermo Spray (TS) spectra, Matrix Assisted Laser Ionization / Desorption (MALDI), Field Desorption (FD) & Plasma Desorption (PD). Tandem Mass Spectroscopy (MS-MS / MS-MS-MS). Analyzer: Magnetic Sector, Quadrupole, Ion Trap, Time-Of-Flight (TOF), Fourier Transform-ion Cyclotron Resonance (FTICR or FTMS).
- 5. Following progress of reactions by spectroscopy:** Diagnostic appearance and disappearance of functional groups in organic compounds and also in characterizing the products.
- 6. Structure elucidation by spectroscopy:** Combined application of UV, IR, NMR, and Mass spectroscopy in the structure elucidation of organic compounds- illustration with the spectra of typical compounds-

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Identify compounds by analysis and interpretation spectral data.
- (ii) Analyze and interpret 1D and 2D NMR spectra.
- (iii) Learn how to use modern mass spectrometry techniques (CI, ESI, FAB, TOF, GC-MS, LC-MS/MS) to find out the molecular mass and structure.
- (iv) Acquire the ability to determine the structure of typical organic compounds using spectroscopic techniques.

Books Recommended

1. Spectroscopic Identification of Organic Compounds: Bassier and Morrill, John Willey and Sons.
2. Spectroscopic Methods in Organic Chemistry: D. H. Williams and I. Fleming, McGraw Hill, New-York.
3. Spectroscopic Analysis: D. L. Pavia, G. M. Lampman and G. S. Kriz
4. Basic One- and Two-Dimensional NMR Spectroscopy: Horst Friebolin, WILEY-VCH, New-York.
5. Mass Spectroscopy: H. C. Hill.
6. Structure Elucidation by NMR in organic chemistry by Eberhard Breitmaier, University of Bonn, Germany.

OC 604 H Natural Products

Learning Objectives

The learning objectives of this course are to

- (i) Give basic knowledge on extraction, isolation & purification of natural products.
- (ii) Develop clear understanding of the chemistry of important natural products like terpenoids, alkaloids, steroids, hormones and natural pigments.
- (iii) Determine the structure of an unknown natural product by chemical and spectroscopic methods.
- (iv) Develop knowledge on biosynthesis of natural products.
- (v) Have an idea about the structure of proteins and nucleic acids.

Course Content

1. **Secondary metabolites:** Their biogenetic groupings and their role in chemotaxonomic classification of plants.
2. **Different pathways of biosynthesis of:** secondary metabolites such as acetate, fatty acid, polyketides-mevalonates, isoprenoids, shikmic acid and amino acids.
3. **Methods of:** plants material analysis and its applications in phytochemical studies.
4. **A general study of :** Isolation, purification, physiological actions and structure elucidation by degradative and different spectroscopic methods, secondary metabolites occurring in plants, with typical structure of terpenoid (zinziberene and phytol), steroids and hormones (sitosterols, ergosterols, lanosterol, sex hormones testosterone, progesterone) carotenoids (β -carotene), alkaloids (morphine and reserpine), vitamins (retinol, cyanocobaltamin) and anthocyanins (cyanin chloride, pelargonin chloride).
5. **Polypeptides and proteins:** Isolation, purification, classification and structure determination with an emphasis on the secondary and tertiary structure of proteins. Composition and functions of insulin, glycoprotein, lipoprotein and proteoglycan.
6. **Lipids:** Importance, functions, classifications and physical characteristics, nonsaponifiable lipids and their biological functions. Glycolipids, VLDL, LDL and HDL.
7. **Nucleic Acids:** Detailed structures f of RNA and DNA, genomics, biosynthesis of proteins.
8. **Industrial utilization of natural resources:** Economic crops as industrial raw material. General uses of chemical methods for value addition and standardization.

Learning Outcomes

Upon completion of this course students will be able to

- (i) Apply the knowledge of extraction, isolation and purification techniques of different natural products like terpenoids and alkaloids.
- (ii) Demonstrate the steps of biosynthesis of carbohydrates, terpenoids alkaloids and steroids.
- (iii) Characterize different terpinoids, carotene flavonoids and alkaloids by chemical as well as spectroscopic methods.
- (iv) Explain the natural pigments like carotenoids, flavonoids etc.
- (v) Discuss the chemistry of different types natural products and know the functions of these natural products.

Books Recommended

1. Organic Chemistry, Vol. 2: Stereochemistry and Chemistry of Natural Products, I. L. Finar.

2. Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis, J. B. Harborne.
3. Secondary Metabolites, J. Mann.
4. Chemistry of Organic Natural Products, Vol. I and II, O. P. Agarwal.
5. Trease and Evans Pharmacognosy, W. C. Evans.
6. Organic Chemistry, F. A. Carey

OC 605 H Organic Pollutants in the Environment

Learning Objectives

The learning objectives of this course are to

- (i) Introduce general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Give general concept on toxicants and their doses, accumulation in organism and excretion.
- (iii) Impart knowledge on pollution by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, fertilizers and their management.
- (iv) Acquaint with the pollution by traditional and modern pesticides, plant growth regulator and their formulation and various actions also food safety and poisoning.
- (v) Gain concepts on integrated pest management to reduce pollution.

Course Content

1. **Degradation of different components of biosphere by environmental pollutants:** A general overview of Interconnections among biosphere, atmosphere, anthrosphere, hydrosphere and geosphere.
2. **Pollution by Hydrocarbons:** Chemical nature, dispersion, evaporation, photooxidation and microbial transformation to the environment; petroleum and aquatic organisms. Biphenyls and polychlorinated biphenyls (PCBs), physical and chemical properties, environmental distribution and behavior. Polycyclic aromatic hydrocarbon: Chemical nature; Occurrence and behavior in the environment; carcinogenicity and toxicity of PAHs; Effect on human health and the natural environment.
3. **Pollutants from Industries, their treatment by chemical, physical, thermal and photochemical method with special references to:** Polymers and Plastic, Soap & Detergents, Chemical & Pharmaceutical and Pulp & Paper industries.
4. **Waste materials and their appropriate disposal by proper chemical & biological treatment of:** municipal waste, domestic, hospital and medical wastes.
5. **Fertilizers:** Nitrogenous, phosphatic and NPK fertilizers, environmental implications of fertilizer; abatement procedure of fertilizer pollution.
6. **Organic pollutants in vegetables, fruits and other food materials:** Insecticides, fungicides, herbicides and their effects on environment and human health. Formulation: Wettable powder, emulsion/solution and fumigants. Mechanism of action and metabolism of pesticides in biological system. Detoxification and their metabolites in the environment.
7. **Insect attractant, repellent and chemosterile, retardant, Plant growth regulators.**
8. **The role of integrated pest management to control pollution: Toxicology:** Introduction to toxicology, Dose-response relationship, Dose & frequency of use, MRL (Maximum Residue Limit) and (Acceptable Daily intake), Integrated pest Management (IPM): Definition, Key components of IPM, Pest control techniques, Reduction of pollution.

Learning Outcomes

Upon completion of the course, the students will be able to

- (i) Demonstrate general idea on common organic pollutants, their source, persistence and effects on living beings.
- (ii) Apply general concept on toxicants and their doses.
- (iii) Manage various pollutions by different hydrocarbons, industrial pollutants, organometallics, hazardous waste, and fertilizers.
- (iv) Assess pollution by traditional and modern pesticides, their formulation also food poisoning and its safety.
- (v) Suggest integrated pest management plan to reduce pollution.

Books Recommended

1. Basic Concept of Environmental Chemistry, D. W. Connell.
2. Fundamental Concept of Environmental Chemistry, G. S. Sodhi.
3. Organic Chemicals: An Environmental Perspective, A. H. Neilson.
4. Environmental Chemistry, A. K. De.
5. Environmental Pollution Analysis, S. M. Khopkar.
6. Environmental Chemistry: Air and Water Pollution, H. S. Stoker and S. L. Seager.
7. Environmental Chemistry, S. E. Manahan.
8. Handbook of Environmental Chemistry Series, O. Hutginger.
9. Environmental Toxicology, M. Stake, M. Mida, M. S. Sethi. S. A. Iqbal, H. Yasuhisa and S. Laguchi.

OC 606 H Organic Synthesis

Learning Objectives

The learning objectives of this course are to

- (i) Provide basic concepts on the strategy for carrying out an organic synthesis.
- (ii) Impart knowledge for developing ability to plan and carry out synthetic experiments independently.
- (iii) Grow critical awareness of advances at the forefront of new methodologies in the synthesis of biologically important organic molecules.

Course Content

1. **A brief treatment of how to design experimental routes for synthesizing a target compound:** Selection of appropriate methods and reagents.
2. **Reaction Intermediates in organic synthesis with particular reference to:** Carbenes, ketenes and enamines.
3. **Organometallic Reagents in organic synthesis:** Utilization of organometallic compounds of alkali metals, alkaline earth metals, boron, tin, silicon, etc.
4. **Oxidation and Reduction methods in synthesis:** Dissolving metal reduction, with hydrazine and its derivatives, oxidation with chromium and manganese compounds, peracids and peroxides, mercuric acetates and selenium dioxide.
5. **Stereoselective synthesis:** Regioselective, diastereoselective and enantioselective synthesis.

6. **Design of Drug synthesis:** Structure activity relationship, use of retrosynthesis in designing synthesis of biologically important organic compounds. Synthesis of some typical medicinal compounds- Ascorbic acid, β -carotene, penicillin, cephalosporin C, prostaglandins ($F_{2\alpha}$ and E_2) and taxol .
7. **Combinatorial synthesis:** Principles, illustration with selected examples, advantages and limitations of combinatorial synthesis.

Learning Outcomes

After completing the course, the students should be able to

- (i) Carry out different synthesis and transformation of the most common functional groups.
- (ii) Describe and apply stereochemical concepts such as chirality, stereoisomerism, and stereoselectivity in relation to chemical transformations
- (iii) .Identify, analyze and evaluate synthetic routes to target molecules by one-group and two group disconnections.
- (iv) Apply organometallic reagents and reactions in organic synthesis.
- (v) Plan and design experimental setups for various types of synthesis of biologically important organic compounds.

Books Recommended

1. Stereoselective Synthesis in Organic Chemistry: Atta-ur-Rahman & Zahir Shah, Springer-Verlag
2. Principles of Organic Synthesis: Norman, Methuen & Co. Ltd.
3. Modern Synthetic Reactions: H. O. House
4. Advanced Organic Chemistry: Reaction Mechanism and Structure: Jerry March
5. Fundamentals of organic reaction mechanisms. J. Milton Harris and Carl C. Wamser
6. Reactive Molecules: Curt Wentrup
7. The disconnection approach : Wiley and Warren, S.
8. Advances in Heterocyclic chemistry : S. F. Dyke.
9. Organic chemistry: Clayden, Greeves, Warren and Wothers.

OC 607 H Carbohydrates and Glycoconjugates.

Learning Objectives

The learning objectives of this course are to

- (i) Give advanced knowledge on monosaccharides and their different structural features in different situations
- (ii) .Impart knowledge on synthesis of glycosides, anhydro- , amino-, and deoxy-sugars and their reactions.
- (iii) Have knowledge on the importance of polysaccharides and their industrial and biological importance.
- (iv) Acquire knowledge for isolation, purification and structural elucidation of complex polysaccharides.
- (v) Review the important polysaccharide derivatives and their applications.

Course Content

1. **Review of:** The study of structure, configuration and conformation of monosaccharides and di saccharides-use of spectroscopic methods in assigning structure and configuration.

2. **Reactions and synthesis of :** Glycosides, amino sugars, deoxy sugars, anhydro sugars, thio sugars, uronic acids and complex carbohydrate derivatives (i.e, Streptose, adenosine triphosphate, ATP).
3. **The biochemistry of monosaccharides:** Catabolic or degradative reactions, interconversion of monosaccharides and synthesis of complex glycosyl compounds.
4. **A comprehensive study on :** Isolation, purification, classification and structure elucidation of polysaccharides from plants, microorganism, algae and seaweeds. Determination of sequence of monosaccharides of complex polysaccharides using spectroscopic and degradative methods with an emphasis on Smith degradation, elimination, nitrous acid deamination, selective oxidation and partial hydrolysis, methylation analysis.
5. **A general study of glycoconjugates involving:** Different reactions of monosaccharides at anomeric and non-anomeric carbon atoms.Synthesis and reactions of glycosides.
6. **Chemistry of polysaccharides of different sources:** Plants, Physical (including spectroscopic) and chemical methods of. Different physical and chemical methods of determination of molecular weight and D. P. of carbohydrate polymer.
7. **General structure of macromolecular carbohydrates** (Primary, secondary and tertiary structure).
8. **Chemistry of dietary fiber:** Sources, classification, methods of isolation, purification and linkage pattern of different dietary fiber.Importance of dietary fiber in prevention of different diseases.
9. **Chemistry of glycoconjugates:** Sources, structure and biological importance of glycoprotein, proteoglycan, different glycolipids and glycosoaminglycans.
10. **Different derivatives of polysaccharides and their technological aspects of applications.**

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the monosaccharide chemistry.
- (ii) Find out route to synthesize different monosaccharide derivatives.
- (iii) Understand the techniques of isolation and purification of complex polysaccharides.
- (iv) .Elucidate the structure of complex polysaccharides using chemicals and spectroscopic means.
- (v) Prepare industrially and biologically important polysaccharides derivatives and use them for suitable purposes.

Books Recommended

1. Advanced in Carbohydrate Chemistry (Series).
2. Methods in Carbohydrates (Series).
3. Monosaccharides - Their Chemistry and Their Roles in Natural Products, P. M. Collins and R. J. Ferrier.
4. Polysaccharides, Vol. I-V, G. O. Aspinal.
5. Principles of Biochemistry, A. L. Lehninger.

Learning Objectives

The learning objectives of this course are to

- (i) Give advanced knowledge on monosaccharides and their different structural features in different situations.
- (ii) Impart knowledge on synthesis of glycosides, anhydro-, amino-, and deoxy-sugars and their reactions.
- (iii) Have knowledge on the importance of polysaccharides and their industrial and biological importance.
- (iv) Acquire knowledge for isolation, purification and structural elucidation of complex polysaccharides.
- (v) Review the important polysaccharide derivatives and their applications.

Course Content

1. **Polymers and polymerization:** Addition (chain reaction) and condensation (step reaction) polymerizations.
2. **Hydrocarbon polymer:** Homopolymers and heteropolymers. Low density and high-density polymers and their properties. Copolymers: Alternating, random, block and graft copolymers. Elastomer, thermoplastic and thermosetting polymers and their properties. Fibre and elastomer.
3. **Mechanism of polymerization:** Radical, cationic and anionic polymerizations, their kinetics, Chain termination, chain transfer, chain retardation and chain inhibition.
4. **Coordination polymerization:** Fluid-bed process, Zeigler-Natta catalysis, mechanism of co-ordination polymerization and its kinetics. Metal oxide catalyzed and Alfin polymerizations. Ring opening polymerization.
5. **Mechanism:** Co-polymerizations and their kinetics.
6. **Configuration of polymers:** Syndiotactic, isotactic and atactic polymers.
7. **Some important polymer:** Production of monomer unit, physical properties and important uses of polymer, polythene, polyvinylchloride (PVC), polystyrene, polybutylene, polybutadiene-styrene, neoprene, polymethyl methacrylate, polyacrylonitrile, polyvinylacetate, poly-terafluoroethylene (PTFE). Polyarnides: Nylon 6, nylon 66, nylon 610, nylon 11 and nylon 12, silk and wool.
8. **Thermosetting resins:** Phenol-formaldehyde, phenol-urea, melamine formaldehyde polymers, their preparation and uses. Epoxy resins and polyurathenes.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the organic polymer chemistry.
- (ii) Find out route to synthesize different organic and synthetic polymers.
- (iii) Understand the mechanism of addition, condensation and coordination polymerization and their kinetics.
- (iv) Elucidate the structure of complex polysaccharides using chemicals and spectroscopic means.
- (v) Prepare industrially and biologically important polysaccharides derivatives and use them for suitable purposes.

Books Recommended

1. Advanced in Carbohydrate Chemistry (Series).
2. Methods in Carbohydrates (Series).
3. Monosaccharides - Their Chemistry and Their Roles in Natural Products, P. M. Collins and R. J. Ferrier.
4. Polysaccharides, Vol. I-V, G. O. Aspinal.
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