

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
Effective for the students admitted from the year 2021 – 2022
SEMESTER – IV
Paper-I: Organic Spectroscopy-II (CH401T (O))

Marks: 70

Learning Objectives:

- ✓ To learn about the basics of ^{13}C NMR, Mass, and 2D NMR spectroscopic techniques.
- ✓ To understand the instrumentation of Mass, types of ionizations, types of analyzers in Mass spectroscopic techniques.
- ✓ To apply the spectroscopy knowledge for the structural elucidation of natural products and stereochemistry of organic compounds.

UNIT-I

14H

^{13}C NMR Spectroscopy:

Types of ^{13}C NMR spectra, Undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. Signal enhancement by Nuclear OVER HAUSER effect. ^{13}C chemical shifts, factors affecting the chemical shifts. Noise decoupled and off-resonance spectra of simple Compounds. Calculation of chemical shifts of alkanes, alkenes, alkynes, and aromatic compounds. Typical examples of CMR spectroscopy –problems.

UNIT-II

14H

Mass Spectroscopy:

Introduction, principles of ionization methods: EI, CI, FDI, PDI, LDI, FAB, TSI and ESI, Types of mass analyzers; Types of fragments- odd electron and even electron containing neutral and charged species (even electron rule), nitrogen rule, molecular-ion peak, base peak, metastable ion, isotopic abundance. High Resolution-MS (HRMS), index of hydrogen deficiency (IHD). Fragmentation of typical organic compounds - hydrocarbons, aromatics, alcohols, alkyl halides, ethers, Carbonyls, carboxylic acids, esters, amines, amides, nitro compounds. General methods of mass spectral fragmentation- β -cleavage, McLafferty rearrangement, retro Diels-Alder fragmentation and ortho effect. Factors affecting fragmentation– Mass spectra related problems.

UNIT-III

10H

2D NMR Techniques:

Principles of 2D NMR, classification of 2D-experiments, 2D-J-resolved spectroscopy. Correlation spectroscopy (COSY), HOMO COSY (^1H - ^1H COSY), COSY of *m*-dinitrobenzene, isopentyl acetate, Hetero COSY (^1H , ^{13}C COSY) Hetero COSY of isopentyl acetate and 4-methyl-2-pentanol, HMQC, HMQC of codeine, long range ^1H , ^{13}C COSY (HMBC), HMBC of codeine and NOESY, NOESY of 9-benzylanthracene, 2-D INADEQUATE experiments.

UNIT-IV**12H**

Spectral characteristics of natural products involving all spectral data: Use of spectroscopic methods UV, IR, ^1H and ^{13}C NMR and Mass spectra in the structure elucidation of natural products. Illustration with suitable compounds like Apigenin (Flavone), Kaempferol (flavonol), Umbelliferone (coumarin), Camphor (Terpenoid), Lawsone (Naphthoquinone), Papaverine (Alkaloid), and Equilenine (steroid).

UNIT-V**10H****Spectral Problems:**

Applications of ^{13}C NMR spectroscopy: Stereochemistry, and reaction mechanisms.

Applications of ^1H NMR spectroscopy: Stereochemistry-Geometrical and optical isomerism.

Spectral Problems involving all spectral data UV-Vis. ^1H NMR, ^{13}C NMR, Mass spectrometry & 2D NMR techniques.

Reference Books:

- 1) Spectrometric identification of organic compounds by R.N.Silverstein & G.C.Bassier (John Willey)
- 2) Spectroscopic methods in Organic Chemistry by Williams and Fleming (McGraw Hill).
- 3) Organic photochemistry by R.O.Kan (Mc Graw Hill)
- 4) Advanced organic Chemistry Reaction Mechanisms and Structure by J March (Mc Graw Hill & Kogshusha).
- 5) Carbon-13 NMR Spectroscopy by J.B. Stothers.

Learning Outcomes:

- ✓ Students can understand the fundamentals of ^{13}C NMR and Mass spectroscopic techniques and apply to investigate the structural information of molecules.
- ✓ It can provide ability to apply the spectroscopy knowledge for the structural elucidation of natural products and stereochemistry of organic compounds
- ✓ It also provides platform for awareness towards ^{13}C NMR and Mass Spectrometry which aims to apply these knowledge towards research.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY

Effective for the students admitted from the year 2021 – 2022

SEMESTER – IV

Paper-II: Organic Synthesis & Reaction Mechanisms-II (CH402T (O))

Marks: 70

Learning Objectives:

- ✓ To learn about the basics of C-C single and double bond formations and Diels-Alder reactions.
- ✓ To learn terminology and develop skills in writing retro-synthetic routes for target molecules with one and two functional groups.
- ✓ To learn different approaches in photochemical and pericyclic reactions.
- ✓ To learn terminology and selectivity in asymmetric synthesis and also apply the approaches in organic synthetic reactions.

UNIT-I

14H

Formation of C-C single & double bonds and Diels-Alder & related reactions:

Formation of C-C single bonds—enamines and related reactions.

Formation of C-C double bonds—Corey-winter olefination, Peterson olefination, Julia olefination, McMurry coupling, Wittig reaction of Phosphorus ylides—stereoselective synthesis of tri and tetra-substituted alkenes.

Diels-Alder and related reactions – diene-dienophile, intramolecular Diels –Alder reactions, Stereochemistry and mechanism Retro Diels – Alder reaction –1, 3-dipolar reactions.

UNIT-II

12H

Synthetic Strategies or Retro Synthetic analysis: Terminology- Target Molecule(TM), synthon, synthetic equivalent, functional group interconversion (FGI), and representation of disconnection of bonds. Linear and convergent synthesis. One group and two group disconnections in simple molecules- Alcohols, Olefins, aryl ketones, α,β -Unsaturated compounds – 1,3 dicarbonyl compounds. synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

UNIT-III

10H

Photochemistry: Photochemistry of olefins—conjugated olefins—Aromatic compounds— isomerisation—additions. Photochemistry of carbonyl compounds – Norrish type I and II reactions –Paterno – Buchi Reaction. Photo reduction, Photochemical rearrangements—Photo Fries rearrangement, Di- π -methane rearrangement.

UNIT-IV

12H

Pericyclic Reactions: Definition, classification, MO theory, Electronic configuration in ground and first excited states of aliphatic conjugated polyene system (upto 4 double bonds).

Electrocyclic Reactions: Mechanism, stereochemistry, PMO, FMO, correlation diagram, Woodward Hoffman rules. **Cycloaddition Reactions:** FMO and correlation diagram methods- (2+2) and (4+2) cycloaddition reactions, stereochemistry. Woodward Hoffman rules.

Sigmatropic Rearrangement: classification, Mechanism by FMO method, Woodward Hoffman rules. Cope, Claisen and Aza-cope rearrangements.

UNIT-V**12H**

Asymmetric Synthesis-II: Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule, and Felkin-Anhmodel. i) Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral Enolates, aza enolates, 1,4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in DielsAlder and Aldol reactions. ii) Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H.; Asymmetric Hydroboration using $(IPC)_2BH$ and $IPCBH_2$.

Reference Books:

- 1) Some Modern methods of synthesis By Caruthers (Cambridge)
- 2) Organic synthesis by Robert & Ireland (Printce Hall of India)
- 3) Designing Organic Synthesis B staurt Warron, John Wiley & Sons
- 4) "Pericyclic reactions a mechanistic study" S.M. Mukheji
- 5) Synthetic approaches in Organic Chemistry " R.K. Bansal Narosa Publications
- 6) Advances in Organic Chemistry – Reaction mechanism and structure" by J. March (Mc Graw Hill).
- 7) 'Organic Photo chemistry and Pericyclic reactions' M.G. Arora Anmol Publications Pvt. Ltd.
- 8) Fundamentals of photochemistry by K.K. Rohatgi–Mukharjee Now Age international publishers.
- 9) Photochemistry by C W S Wells.
- 10) Organic Photochemistry by Turro.
- 11) Molecular Photo chemistry by Gilbert & Baggo.
- 12) Organic Photo chemistry by D Coyle.
- 13) Asymmetric synthesis by Nogradi.
- 14) Asymmetric organic reactions, J. D. Morrison and H. S. Moscher.
- 15) Principles of Asymmetric synthesis, R. E. Gawley and J. Aube, 2nd Ed., Elsevier, 2012.

Learning Outcomes:

- ✓ Students understand the basics of C-C single and double bond formations and Diels–Aider reactions.
- ✓ Students learnt the terminology and develop skills in writing retro-synthetic routes for target molecules with one and two functional groups.
- ✓ Students learnt different approaches in photochemical and pericyclic reactions
- ✓ Students are able to understand the terminology and able to know selectivity in asymmetric synthesis and also able to apply the approaches in organic synthetic reactions.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY

Effective for the students admitted from the year 2021 – 2022

SEMESTER – IV

Paper-III: Chemistry of Antibiotics and Drugs (CH403T (O))

Marks: 70

Learning Objectives:

- ✓ To know the basics on antibiotics, their importance and various drugs in medicinal chemistry.
- ✓ To know the chemistry of structures and synthesis of some antimalarials, sulpha drugs, antiseptic and antifungals.
- ✓ To know the classification of herbal drugs and their therapeutic efficacy and isolation.

UNIT-I

12H

Antibiotics:

Synthesis of penicillin-G, ampicillin, amoxicillin, chloramphenicol, cephalosporin. Streptomycin, tetracyclines, Terramycin, aureomycin, gramicidin.

UNIT-II

12H

Drugs and Medicinal chemistry:

Anticancer Agents: Synthesis & Activity relationship of Taxol, Vinblastine, Vincristine, Camptothecin.

CNS stimulants: Strychnine (CNS activity only), caffeine, Nicotine; CNS depressants, General anesthetics, mode of action of Sedatives & Hypnotics.

UNIT-III

12H

Antimalarials: Paludrin – quinacrin – chloroquin – camoquin – pamaquin – ontoquine.

Sulpha drugs: Sulphanilamide – Dihydrocurprine – Prontosil

UNIT-IV

12H

Antiseptics and Antifungal agents

Antiseptics: Common types, triclosan, aminacrine hydrochloride. Antiseptics Vs Disinfectants- Properties, Mechanism of action, classification

Antifungal agents: 1,8-dihydroxyanthranol – griseofulvin.

UNIT-V

12H

Herbal Drugs: i) Classification of herbal drugs- Pharmacological and Chemical classification. ii) Adulteration and evaluation of drugs. iii) Different chemical groups of Herbal drugs- Alkaloids, Terpenoids, Glycosides, Volatile oils, Isolation of volatile oils, Tannins, and carbohydrates. iv) Herbal drugs and their therapeutic efficacy. Isolation of- Laxative-Aloe-

emodin from Aloes. Anti-diabetics- Neem oil (Neem); Anti-malarial- Quinine (cinchona); Anti-hypertensive- Reserpine (rauwolfia).

Reference Books:

- 1) Introduction to Medicinal Chemistry – Wiley VCH
- 2) Text Book of Organic Medicinal and Pharmaceutical Chemistry, Wilson and Gisvild, (ed Robert F. Dorge)
- 3) An introduction to drug design by SS Pandeya
- 4) Burger's Medicinal Chemistry and drug discovery Vol.I by (Ed) ME Wolff – John – Wileyby A. Burger
- 5) The Organic Chemistry of drug design and drug action by RB Silverman, Academic press
- 6) Principles of Medicinal Chemistry by William O. Foye, Lea & Febiger, Philadelphia/London, 1989.
- 7) Natural products. By P.S.Kalsi
- 8) Medicinal chemistry. By Chatwal.- And By Ashtoshkar.
- 9) Chemistry of Drugs. By V.N.Ivers.
- 10) May's chemistry of synthetic drugs. Hand Book of Reagents for organic synthesis. By Reich,Rigby
- 11) Top Drugs: The synthetic routes. J.Saunders
- 12) Organic natural products By Barton and Ollis
- 13) Organic natural products by OP Agarwal
- 14) Organic natural products By Barton and Ollis.

Learning Outcomes:

- ✓ Students understand the basics on antibiotics, their importance and various drugs used in medicinal chemistry.
- ✓ Students are able to understand chemistry and synthesis of antimalarials, sulpha drugs, antiseptic and antifungals used in medicine.
- ✓ Students can identify the classification of herbal drugs in various types and understand their therapeutic efficacy and isolation methods.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
Effective for the students admitted from the year 2021 – 2022
SEMESTER – IV
Paper-IV: Advanced Organic Chemistry (CH404T (O))
Core Elective-II (CE-II)

Marks: 70

Learning Objectives:

- ✓ To introduce novel named reactions in modern organic synthesis.
- ✓ To know importance and principles of green chemistry, and microwave assisted reactions.
- ✓ To know the role of Nanochemistry in various fields and synthesis methods (Solid and Gase phase).
- ✓ To introduce green chemistry and microwave assisted reactions.
- ✓ To know use of organoboranes and organosilanes in synthesis.
- ✓ To introduce supramolecular chemistry and to know the mechanism of building blocks.

UNIT-I

12H

Advanced named Reactions in Organic Synthesis:

Baylis-Hillmon reaction, RCM Olefin metathesis, Grubb's catalyst, Mitsunobu reaction, Suzuki Coupling, Heck Coupling, Stille Coupling, Sonagashia, Coupling, Negishi Coupling, Hiyama Coupling, Buchwold – Hartwig Reaction, Click Reaction.

UNIT-II

10H

Nano Chemistry

Introduction, Carbon Nanotubes: structure of single and multi wall carbon nanotubes, synthesis-solid and gaseous carbon source-based production techniques, synthesis with controlled orientation. Growth mechanism of carbon nanotubes-catalyst free growth, catalyst activated growth, nano buds, nanotorus properties-general, adsorption, electronic & optical, Mechanical and reactivity. Defects, Toxicity Applications.

UNIT-III

14H

Green Synthesis:

Introduction, Principles, Green solvents- supercritical fluids, water, ionic liquids and PEGs as green solvents for organic reactions. Examples of green reactions-synthesis of Ibuprofen, Clean Fischer-Indole synthesis comparison of the above with conventional methods.

Microwave Organic Synthesis: Introduction, Applications: Microwave-assisted reactions in water (oxidation of toluene to benzoic acid, oxidation of alcohols); organic solvents (Diels-Alder reaction and Decarboxylation); solvent-free reactions (solid state reaction)-Michael addition and Knoevenagel reaction), multistep V/s single pot synthesis.

UNIT-IV

12H

Organoboranes and Silanes:

Organoboranes: Synthetic applications of organoboranes – protonolysis, oxidation, carbonylation Reaction of alkenyl borane – enantioselective synthesis of secondary alcohols from alkenes.

Organosilanes: Synthesis of organosilanes, general features of carbon-carbon bond forming reactions of organosilicon compounds, addition reactions with aldehydes and ketones, acylation reactions, conjugate addition reactions.

UNIT-V

12H

Supramolecular Chemistry: Introduction - the meaning of supramolecular chemistry, phenomenon of molecular recognition and their quantification Building blocks of supramolecular chemistry - acyclic receptors for neutral and charged guests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbituril and cyclodextrins.

Reference Books:

- 1) New trends in green Chemistry by V.K.Ahluwalia
- 2) Organic synthesis by Robert & Ireland (Printce Hall of India)
- 3) Designing Organic Synthesis B staurt Warron, John Wiley & Sons
- 4) Green chemistry, *V.K.Ahluwalia*, Ane books.
- 5) P.T. Anastas and J.C.Warner *Green chemistry*, Oxford.
- 6) G.A.Ozin, A.C. Arsenault *Nano chemistry*, RSC.
- 7) Diwan, Bharadwaj, *Nanocomposites*, Pentagon.
- 8) V.S.Muralidharan A.Subramania, *Nanoscience and Technology*, Ane Books.
- 9) J.W Steed and J.L Atwood, *Supramolecular chemistry*, John Wiley & Sons, Ltd. New York.
- 10) Piet W. N. M. van Leeuwen, *Supramolecular Catalysis*, Wiley-VCH Verlag GmbH & Co.
- 11) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons.
- 12) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House.

Learning Outcomes:

- ✓ Students able to understand novel named reactions and applications in modern organic synthesis.
- ✓ Students understand the importance and principles of green chemistry, microwave assisted reactions and know applying the green synthesis to organic reactions.
- ✓ Students know current importance of Nanochemistry in various fields and their synthetic methods (Solid and Gase phase).
- ✓ It provides the knowledge of usinf organoboranes and organosilanes in synthesis.
- ✓ Students understand requirements of guest and host and formation of building blocks of supramolecular chemistry.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
Effective for the students admitted from the year 2021 – 2022
SEMESTER – IV
Paper-V: Forensic Science - In Solving Crime (CH405T)
Other Elective (OE-II)

Marks: 70

Learning Objectives:

- ✓ The significance of Forensic science to human society.
- ✓ The fundamental principles and functions of Forensic science.
- ✓ The divisions in a Forensic science laboratory.
- ✓ The various steps to be taken to thoroughly record the crime scene.
- ✓ The legal importance of chain of custody.

UNIT-I

12H

Introduction to Forensic Science: Need and functions of Forensic science. Historical aspects of Forensic science. Development of Forensic Science Laboratories. Definitions and concepts in Forensic science. Basic principles of Forensic science. Scope of Forensic science. Governing principals of Forensic Science. Forensic Science in Indian scenario. Admissibility in Indian Courts. Frye standard and Daubert standard.

Unit-II

12H

Divisions of Forensic Science

Branches of Forensic science and their importance. Hierarchical set up of various Government Forensic Science Laboratories.

Forensic Evidences: Concise of Forensic Physical, Biological, Chemical and Psychological evidences, Medico-Legal Cases. Legal and Scientific problems. Forensic intelligence and Interviews.

UNIT-III

12H

Crime Scene

Types of crime scenes. Safety measures at crime scenes. Role of First Responding Officer. Coordination between police personnel and Forensic scientists at crime scenes. The evaluation of 5Ws (who? what? when? where? why?) and 1H (how?)

UNIT-IV

12H

Police and Forensic Science

Relationship between police and forensic expert, Role of Police at the Crime scene, scientific help at crime scene, Importance of Chain of custody, handling of various types of crime scenes by police, forensic teaching of police personals, forensic case documentation by Police, Technological Advance and Police, Mobile device forensics, Role of Media, Human Rights Commission & Criminal Justice System.

UNIT-V

12H

Administration and Organizational Setup:

DFSS, CFSL, GEQD, SFSL, RFSL, MFSL, FPB, NICFS, CDTS, NCRB, BPR&D, Qualifications and duties of Forensic Scientists Academic centres of education and research: Indian and Academy of Forensic Science, American Board of Forensic Science, American Board of Forensic Odontology, Bureau of Alcohol Tobacco and Firearms, Interpol and FBI, Australian Academy of Forensic Sciences. Forensic Science in India: Teaching Courses and Research fields in Forensic Science, Scope and jobs in Forensic Science.

Learning Outcomes:

- ✓ The definition and difference between Forensic Science and Criminalists.
- ✓ The major contributors to the development of Forensic Science.
- ✓ Importance of physical evidence.
- ✓ To Learn Forensic Technology solving crimes with advanced technology
- ✓ Explain the steps typically required to maintain appropriate health and safety standards at the crime scene.

PRACTICAL SYLLABUS

Course: M.Sc.; Specialization: ORGANIC CHEMISTRY

Semester: IV; From Admitted Batches: 2021-22

Practical-I: Analysis of Binary Organic Mixture

Max. Marks: 70 (15QA+45Prac.+10Rec.)

Part I: One theory question relating to any topic out of four semesters or any practical or as wish by the examiner. 15M

Part II: Two component organic mixture analysis 45M

The mixture separation should be done by chemical methods and their identification by chemical reactions. Separation is based on solvent selection like ether, dil HCl, 5 % aqueous NaHCO₃, and Na₂CO₃ solutions, checking the purity of two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), functional groups, preparation of crystalline derivatives and identification by referring literature data.

(The student must be given trained in at least eight mixtures with different functional groups)

Note: 1. For University examinations the student has to submit at least one derivative for each individual component. Examination- Duration: 9 hours.

Part-III: Record submission 10M

Course: M.Sc.; Specialization: ORGANIC CHEMISTRY

Semester: IV; From Admitted Batches: 2021-22

Practical-II: Project Work/Review of Literature/Spectral Problems

Max. Marks: 100

Title Selection: 1) Project Work / 2) Review of Literature (only on respective Chemistry specialization topics) / 3) Spectral Problems

1) Project Work: For University students- Project Work / Internship is compulsory and have to submit a dissertation containing Back ground of the work, Experimental, Results and Discussion and Summary.

In respect of affiliated Colleges-Project work is optional for only colleges having doctorate degree faculty and students may opt for project work and others have to select *Spectral Problems paper/Review of literature* on core topics only.

2) Review of Literature: The students opted for Review of literature paper must be assigned a latest topic in chemistry and the students have to submit a dissertation (40-50 pages) covering all the latest literature on the topic assigned. The candidate will be assessed at the time of the conduct of final practical examination of the semester taking into consideration of dissertation and viva-voce on the topic chosen for Review of Literature paper.

3) Spectral Problems: For students who selected spectral problems will be given spectra of two different compounds for structural elucidation along with Viva-voce. (A minimum of 10 representative examples should be studied in regular practical hours).

Course: M.Sc.; Specialization: ORGANIC CHEMISTRY

Semester: IV; From Admitted Batches: 2021-22)

Practical-III: Comprehensive Viva-voce

Max. Marks: 50 M

The students will be analyzed with questions covering all four semester topics.