ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
Effective for the students admitted from the year 2021 – 2022

SEMESTER – III
Paper-I: Organic Spectroscopy-I (CH301T (O))

Max. Marks: 70 M

Learning Objectives:

- ✓ To learn about the basics of various spectroscopic techniques.
- ✓ To understand the instrumentation of UV, IR, NMR, ESR spectroscopic techniques.
- ✓ To apply the spectroscopy knowledge for the structural elucidation of organic molecules.

UNIT-I **14H**

UV-Vis Spectroscopy:

a) **UV Spectroscopy**: Energy transitions – Simple chromophores – UV absorption of Alkenes – polyenes unsaturated cyclic systems – Carbonyl compounds, α,β-unsaturated carbonyl systems - Woodward Fieser rules – aromatic systems – solvent effects – geometrical isomerism – acid and base effects – typical examples – calculation of λ_{max} values using Woodward - Fieser rules.
b) **ORD:** Theory of optical rotatory dispersion, α-Axial haloketone rule and octant rule – Application of these rules in the determination of absolute configuration of cyclohexanones, decalones and cholestanones.
c) **Circular Dichroism:** Principle – positive and negative cotton effects – Absolute configuration.

UNIT-II **12H**

Infrared Spectroscopy (FT-IR): Fundamental modes of vibrations – Stretching and bending vibrations – overtones, combination bands and Fermi resonance, factors influencing vibrational frequencies, hydrogen bonding – fingerprint region and its importance – Study of typical group frequencies for – CH, -OH, -NH, -CO-NH_2, -CC, -CHO, -CO and aromatic systems.
Application in structural determination –Simple problems.

UNIT-III **14H**

^{1}H NMR spectroscopy:

a) Magnetic properties of Nuclei, Nuclear resonance, Fourier Transformation and its importance in NMR. Equivalent and non-equivalent protons, The chemical shift and its importance, calculation of chemical shift, factors affecting the chemical shifts such as electronegativity and anisotropy, effect of deuteration, Signal integration, Spin-spin coupling: vicinal (Karplus relationships), germinal and long range. Coupling constants (*J*) and factors affecting coupling constants. –Shielding and deshielding mechanisms in acetylene carbonyl and Benzene, anisotropy –Spin-Spin Interactions related to first order and higher order spectra (AB, A_2; AB_2, ABX, ABC, AMX) –temperature dependence spectra, Hydrogen bonding. Nuclear Overhauser effect (NOE).
b) Interpretation of NMR spectrum of a given compound leading to identification –typical examples of PMR spectroscopy.

UNIT-IV **10H**

Electron Spin Resonance Spectroscopy (**ESR**):

a) Basic Principles, Comparison of NMR & ESR. Determination of 'g' value, Factors affecting the 'g' value. Isotropic and Anisotropic constants. Splitting, hyperfine splitting coupling constants. Line width, Zero field splitting, and Kramer degeneracy. Crystal field splitting, Crystal field effects.

b) **Applications:** Detection of free radicals; ESR spectra of
(a) Methyl radical ($CH_3^{\cdot}$), (b) Benzene anion ($C_6H_6^{-}$).

UNIT-V **10H**

Common Problem on UV-Vis, FT-IR, and ^{1}H NMR:

a) Problems involving individual spectral methods – UV, IR, and PMR
b) Problems involving combined any two of UV, IR, and PMR
c) Problems involving all three UV, IR, and PMR spectral data.

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).

Learning Outcomes:

- ✓ Students can understand the fundamentals of spectroscopic techniques and apply to investigate the structural information of molecules.
- ✓ It can provide a platform to get the awareness towards UV, FTIR, ^{1}H NMR and ESR Spectrometry which aims to apply this knowledge towards research.

ACHARYA NAGARJUNA UNIVERSITY
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SEMESTER – III
Paper-II: Organic Synthesis & Reaction Mechanisms-I (CH302T (O))

Marks: 70

Learning Objectives:

- ✓ To learn about the basics of tools required for determining reaction mechanisms
- ✓ To develop simple skills in writing mechanism of organic reactions.
- ✓ To understand different radical reactions involving additions, substitutions, and decompositions and their mechanisms
- ✓ To learn different approaches and reagents of various oxidation and reduction processes in organic synthesis and also their mechanisms
- ✓ To learn terminology and selectivity in asymmetric synthesis and also apply the approaches in organic synthetic reactions.

UNIT-I **10H**

Methods for Reaction Mechanism by Kinetic & Non-Kinetic studies

Kinetic studies: Kinetics of reaction, Energy profile diagram, Intermediate versus transition state, Reaction rate and rate limiting step.

Non-Kinetic studies Identification of products, testing possible intermediates, trapping of intermediates, Cross over experiments, Isotopic labeling.

UNIT-II **10H**

Free Radicals

Free radicals and their reactions-Introduction to radical reactions, Addition of halogens, Hydrogen halides. Substitution reactions- Halogenation, Aromatic substitution, Sandmayer reaction, Autooxidation, Decomposition of dialkyl and diacyl peroxides.

UNIT-III **14H**

Oxidations

Introduction: Different Oxidative processes.

Hydrocarbon: Alkenes, aromatic rings saturated C-H groups (activated and unactivated), Alcohols, diols, aldehydes, Ketones, Carboxylic acids, Amines, hydrazines, sulphides. Oxidations with ruthenium tetroxide iodobenzene diaccetate and Tl(III) nitrate, Lead tetra acetate, SeO_2, MnO_2 Ag_2CO_3, peracids.

Oxidation of C=C perhydroxylation using $KMnO_4$, OsO_4, peracids.

UNIT-IV **14H**

Reductions

Introduction: Reductive process Hydrocarbons: Alkanes, alkenes, alkynes, and aromatic rings

Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Nitro, nitroso, azo and oxime group Hydrogenolysis. Catalytic hydrogenations, Reduction by dissolving metals, Reduction with metal and acid. Reduction with metal in liquid ammonia (Birch reduction).

Reduction by hydride transfer reagents Aluminium alkoxide, LiAlH4, NaBH4, Diisobutyl aluminium hydrides –Sodium cyano borohydride ,tryalkyl borohydirdes – Reduction with diimide.

UNIT-V **12H**

Asymmetric Synthesis-I

Terminology: Topocity in molecules Homotopic, stereo Heterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re, and Si.

Selectivity in synthesis: Stereo specific reactions (substrate stereoselectivity). Conditions Stereo selective reactions (product stereoselectivity): Enantio selectivity and diastereoselectivity.:

Analytical methods: % Enantiomer excess, optical purity, % diastereomeric excess.

Reference Books:

1) Mechanism and structure in Organic Chemistry " E.S.Could Henry – Holt and Co, Newyork,
2) Advances in Organic Reaction mechanism and structure J. March (McGrew Hill),
3) Aguide Book to Mechanism in Organic Chemistry" by P.Sykes,
4) Synthetic approaches in organic chemistry by R.K.Bansal (Narosa Publications).
5) Some modern methods of synthesis by Carruthers (Cambridge).
6) Asymmetric synthesis by Nogradi,
7) Asymmetric organic reactions by it) Morrison and HS Moschcr,
8) Stereo differentiating reactions by Izumi.

Learning Outcomes:

- ✓ Students can understand the fundamental tools required for the determination of reaction mechanisms.
- ✓ Students can able to apply the reagents and approaches for various synthetic reactions involving oxidations and reductions
- ✓ The knowledge on asymmetric synthesis provides a platform for carryout various stereo chemical reactions wherever necessary to apply towards research.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
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SEMESTER – III
Paper-III: Alkaloids, Terpenoids, Quinones and Phenothiazines (CH303T (O)

Marks: 70

Learning Objectives:

- ✓ To learn about definition and importance of various alkaloids.
- ✓ To know the structure elucidation and synthetic methods of important alkaloids.
- ✓ To know the classification of terpenoids, isoprene rule, structures and their natural sources.
- ✓ To know the structure characterization and synthesis of quinines and phenothiazines.

UNIT-I **14H**

Alkaloids-I: Definition, General methods of identification of alkaloids - nomenclature – occurrence – isolation – chemical tests for identification - general methods of structural elucidation – degradation – classification based on nitrogen heterocyclic ring – role of alkaloids in plants.

a) Structure and synthesis of Atropine, Caffeine.
b) Quinoline alkaloids: Chemistry and synthesis of Quinine, Cinchonine, and their stereochemistry.

UNIT-II **12H**

Alkaloids-II:

a) Isoquinoline-Morphine Group Alkaloids: Papaverine, Hydrastine, narcotine, canadine, Coclawrine, Morphine, Codeine, emetine, Apomorphine, Glaucine
b) Stereochemistry of emetine, and morphine alkaloids.
c) Biogenesis of alkaloids.

UNIT-III **10H**

Alkaloids-III:

a) Indole alkaloids: Reserpine, strychnine, brucine, lysergic acid, erogotamine
b) Structure, stereochemistry, synthesis and biosynthesis of Ephedrine, Conine and nicotine.

UNIT-IV **10H**

Terpenoids: Classificaiton, sources, isolation, synthesis and stereochemistry with special reference to zingiberene, santonin, eudesmol, abietic acid, Biosynthesis of terpenoids.

UNIT-V **14H**

Quinones and Phenothiazines:

Quinones: Identification of quinones, Lapachol. Chrysophenol and Physcion-chemistryand synthesis.

Phenothiazines: Classification, pharmacological properties of phenothaizines, general methods of synthesis of phenothiazines with reference to Promazine, Prochlorperazine and Thioriazine.

Reference Books:

1) Alkaloids by K.W. Bentley Vols. I & II.
2) Text Book of Organic Chemistry I.L. Finar Vol. II 3.An introduction of alkaloids by G.A. Swain,
3) Naturally occurring quinines – R. H. Johnson Vol. I & II, Academic Press, London.

Other References:

1) Chemistry and physiology of alkaloids by Manske Vol. I & II, VII
2) Medicinal Chemistry by A. Burger
3) Isoquinoline Alkaloids by M.Shamma
4) Heterocylclic Chemistry by JA Joule etal., Chapman – Hall.

Learning Outcomes:

- ✓ Students can understand the definitions and importance of various alkaloids
- ✓ Students can understand the structure elucidation and also know the synthetic processes application and synthetic methods of studied alkaloids
- ✓ Basic ideas of isoprene rule, terpenoids classification, their natural sources, synthesis.
- ✓ Students can understand the structure characterization and synthesis of quinones and Phenothiazines.

ACHARYA NAGARJUNA UNIVERSITY
M.Sc. FINAL YEAR CHEMISTRY
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SEMESTER – III
Paper-IV: Chemistry of Natural Products-I (CH304T (O))
Core Elective-I (CE-I)

Marks: 70

Learning Objectives:

- ✓ To know about classification and general methods of synthesis of various flavonoids.
- ✓ To know the structures and synthesis of Fat and water soluble vitamins.
- ✓ To know the classification of harmones, and synthesis of some steroidal and non-steroidal harmones.
- ✓ To know about aminoacids, proteins, enzymes, cofactors and prostaglandins.

UNIT-I **12H**

Flavonoids and Prostagladins

Flavonoids: Classificaiton, sources, isolation, general methods of synthesis of flavones, flavanones, flavonols. Chemistry and synthesis with special reference to quercetin and kampferol.

Prostaglandins: Prostaglandins with special reference to PGE and PGF

UNIT-II **12H**

Vitamins

Fat Soluble Vitamins: Chemistry, Synthesis & biosynthesis of vitamin A_1, vitamin E (α, β, γ, δ-tocopherols) and vitamin K

Water soluble Vitamins: Chemistry, Synthesis, and biosynthesis of B_1 and C

UNIT-III **12H**

Steroidal Hormones

Chemistry & synthesis of equilenine, oestrone, progesterone, androsterone, testosterone, cortisone.

Non-steroid hormones: Chemistry & synthesis of thyroxin, epinephrine, and oxytocin.

UNIT-IV **12H**

Amino Acids: Classification of amino acids. Specific methods of preparations –Malonic ester synthesis and Erlenmeyer azlactone synthesis. Isoelectric point.

Proteins: General nature of proteins – annealing, Biuret reaction, Ninhydrin test. Classification of proteins. Merrifield solid phase peptide synthesis. Primary, secondary, tertiary, and quaternary structure of proteins.

a) Enzymes: classification, kinetics, and mechanism of enzyme action
b) Coenzymes and cofactors: NAD FAD folic acid citric acid cycle.

UNIT-V **12H**

Insecticides

Naturally occurring insecticides: Introduction, general properties, sources, isolation, synthesis, and stereochemistry of Pyrethrin I and II; Jasmolin I & II; Structure activity relationship (SAR) studies and biosynthesis of pyrethrins

Rotenoids: Chemistry and synthesis of rotenone

Isobutylamines: Chemistry and synthesis of anacyclin, and spilanthol .

Minor insecticides of plant origin: Pachyrrhizin and custard-apple.

Reference Books:

1) Steroids by Fieser and Fieser,
2) The Vitamins by S.F. Dykes,
3) The Natural Pigments by K.W. Bentley,
4) Biological Chemistry by Holum,
5) Organic Chemistry Vol.II by I.L.Finar,
6) Naturally occurring insecticides by M. Jacobson and D.G. Crosby, Marcel- Decker Inc, New York.
7) General Organic and Biochemistry by F.A. Bettelheim and Jerry March, Saunders College, Publishing.

Further Study:

1) The terpenoids by Simonsen,
2) The steroids by Shoppee,
3) Chemistry of Carbon compounds by Rodd.

Learning Outcomes:

- ✓ Students can understand the classification and general methods of synthesis of various flavonoids.
- ✓ Students can understand the synthesis of fat and water soluble vitamins
- ✓ To know the classification of harmones, and synthesis of some steroidal and non-steroidal harmones
- ✓ Students can able to understand functions, structures and synthesis amino acids, proteins, enzymes, cofactors and prostaglandins
- ✓ Students able to understand different types of naturally occurring insecticides and their specific and commercial importance.

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M.Sc. FINAL YEAR CHEMISTRY
Effective for the students admitted from the year 2021 – 2022

SEMESTER – III
Paper-V: Applications of Synthetic Products (CH305T)
Other Elective –I (OE-I)

Marks: 70

Learning Objectives:

- ✓ To know the basics of dyes, drugs and also their importance.
- ✓ To know about the production and working of soaps, detergents and formulations of cosmetics.
- ✓ To know about flavours, sweeteners, insecticides, and their applications.
- ✓ To know about explosions and polymer types.

UNIT-I **12H**

Dyes: Colour and constitution, classification, dyeing method, and their industrial importance.

Drugs: Basic concepts, classification, sources, the requirement of an ideal drug.

UNIT-II **12H**

Synthetic Drugs: Structure and medicinal properties.

Sulphanilamide: An example of sulpha drug - paracetamol, aspirin, oil of wintergreen; Mephensin.

A muscle relaxant; Ibuprofen – an anti-inflammatory drug; L-dopa-cures Parkinson's disease;

UNIT-III **12H**

Soaps and Detergents: Production and their cleansing action.

Liquid crystals and their applications. Surfactants

Cosmetics: Detailed study of formulations and manufacturing of cream and lotions, lipstick and nail polish, shampoos, hair dyes, and toothpastes.

Flavours: Natural flavouring materials and classification.

UNIT-IV **12H**

Sweeteners: Natural and Synthetic sweeteners.

Pesticides: Introduction, Classification, Applications and their effect on the environment.

Insecticides: Introduction, Classification, Applications and their effect on the environment.

Explosives: Introduction, RDX, Gun Powder.

UNIT-V **12H**

Polymers: Introduction, biodegradable and non-biodegradable polymers and their industrial importance, plastics (uses and effects on environment), natural and synthetic rubbers, polyamides, and polyesters like nylon, decron, terelyne. Thermoplastics–Poly carbonates, Poly acrylates in lens applications, Polyurethanes, and conducting polymers.

Reference Books:

1) I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.742.
2) K. Albert, L Lehninger, D. L. Nelson, M.M. Cox, Principles of Biochemistry, CBZ Publishers, 1st Edition, New Delhi, 1993.
3) Harper's Biochemistry, Ed. R. Harper, 22nd Edition, Prentice Hall Press, New York, 1990.
4) Encyclopedia of Chemical Technology – Kirck – Othmer Series.
5) Harper's Review of Biochemistry – P.W. Martin, P.A. Mayer & V.W. Rodfwell, 15th Edition, Maurzen Asian Edition, California, 1981.
6) Polymer Science, Gowarikar.
7) Industrial Chemistry, B.K. Sharma.

Learning Outcomes:

- ✓ The students able to understand dyes and their industrial importance.
- ✓ The students understand the cleansing action of soaps, manufacture of cosmetics and use of flavours and sweetness.
- ✓ The students able to understand effects of pesticides and insectides to the environment.
- ✓ The students understand about explosive materials and preparation & use of polymers in industries.

PRACTICAL SYLLABUS

Course: M.Sc. Specialization: ORGANIC CHEMISTRY

Semester: III; From Admitted Batches: 2021-22

PRACTICAL-I: Multistage Organic Synthesis

(Any five experiments must be carryout) Max. Marks: 70 (60 Prac. + 10 Rec.)

Expt-1: Synthesis of paracetomol from benzene

Step 1: Benzene to Nitrobenzene (Nitration)

Step 2: Nitrobenzene to N-phenyl hydroxylamine (reduction)

Step 3: N-phenyl hydroxyl amine to *p*-aminophenol (Rearrangement)

Step 4: *p*-amino phenol to *p*-hydroxy acetanilide/paracetomol(acetylation)

Expt-2: Synthesis of *o*-chlorobenzoic acid from phthalic acid

Step 1: Phthalic acid to phthalic anhydride (Dehydration)

Step 2: Phthalic anhydride –phthalic amide (Amide formation)

Step 3: Phthalmide- Anthranilic acid (Hoffman's Bromamide reaction)

Step 4: Anthranilic acid -*ortho*-chloro benzoic acid

Expt-3: Synthesis of sulpha drug from aniline

Step 1: Aniline to acetanilide

Step 2: Acetanilide to *p*-acetamide benzene sulphonyl chloride (sulphonation)

Step 3: *p*-acetamide benzenesulphonylchloride to *p*-acetamide benzenesulphonamide (s-amination)

Step 4: *p*-acetamide benzene sulphonamide to *p*-amino benzenesulphonamide(hydrolysis)

Expt-4: *m*-Chloro-nitrobenzene from nitrobenzene

Step 1: Nitro benzene to *m*-dinitro benzene (nitration)

Step 2: *m*-dinitrobenzene to *m*-nitro aniline (partial reduction)

Step 3: *m*-nitro aniline to *m*-nitrodiazoniumchloride (diazotization)

Step 4: *m*-nitrodiazoniumchloride to *m*-Chloro-nitrobenzene (sandmayers reaction)

Expt-5: Synthesis of *p*-bromo benzanilide from benzophenone

Step 1: Benzophenone to benzopenone oxime (Addition)

Step 2: Benzophenone oxime to benzanilide (Beckman's rearrangement)

Step 3: Benzanilide to *p*-bromobenzanilide) (bromination)

Expt-6: Synthesis of Methyl orange from aniline

Step 1: Aniline to sulphonic acid (sulphonation)

Step 2: sulphonic acid to Diazonium chloride (diazotization)

Step 3: Diazonium chloride to methyl orange (coupling reaction)

Expt-7: Synthesis of Acridone from Anthranilic acid

Step 1: Anthraninilc acid to o-chlorobenzoic acid (Diazotosation followed by sand mayer's reaction)

Step 2: o-chlorobenzoic acid to N-phenyl anthranilic acid (Substitution)

Step 3: N-phenyl anthranilic acid to acridone (Cyclisation)

Note: All the students must submit the TLC for all the stages of preparation and a photo copy must be pasted in records.

References:

1. Practical Organic Chemistry A.I.Vogel (Longmans)
2. Text Book of practical organic Chemistry F.G.Mann & B.C. Sanders.
3. A Manual of Practical Organic Chemistry Day Sitaramam & Govindachari
4. Organic Experiments L.F.Fieser.
5. Practical Organic Chemistry H.T.Openshaw
6. Systematic Identification of Organic Compounds, P.L.Shriner, R.C.Fuson & D.Y.Curtin.
7. Identification of Organic Compounds N.D.Cheronis & J.B.Entrilkin
8. Advanced Organic Synthesis by R.S.Monson Academic Press

Note: For University Practical Examination: Duration: 9 hours.

Course: M.Sc., Specialization: ORGANIC CHEMISTRY

Semester: III; From Admitted Batches: 2021-22

PRACTICAL–II :: Organic Estimations

(Any six experiments must be carryout) Max. Marks: 70 (15 QA+45 Prac.+10 Rec.)

Part I: One theory question either relating to spectral characterization or any practical or as wish by the examiner. 15M

Part II: The following Estimations/Isolations 45M

Expt. 1: Estimation of hydroxyl group by acetylation or pthalation method

Expt. 2: Estimation of phenol (bromination method)

Expt. 3: Estimation of aniline (Bromination method)

Expt. 4: Estimation of carbonyl groups (Hydrazone formation method)

Expt. 5: Estimation of sugars –glucose and sucrose by using Fehlings solution

Expt. 6: Determination of iodine value of oil or fat

Expt. 7: Determination of saponification value of oil or fat

Expt. 8: Estimation of vitamin 'C' in lime juice.

Expt. 9: Isolation of caffeine from tea/coffee sample.

Part-III: Record Submission **10M**

For University Practical Examination: Duration: 9 hours