

ACHARYA NAGARJUNA UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III
PAPER-I: ORGANIC SPECTROSCOPY-I (R22OC31)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

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.
- ✓ To understand the interpretation of NMR Spectroscopy of given compound.
- ✓ To learn and solve the spectral problems of UV-IR & PMR.

UNIT-I

14H

UV-Visible 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-NH₂, -CC, -CHO, -CO and aromatic systems.
Application in structural determination – Simple problems.

UNIT-III

14H

¹H 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, A₂; AB₂, ABX, ABC, AMX)-temperature dependence spectra, Hydrogen bonding. Nuclear Overhauser effect (NOE).

- b) Applications: 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 ^1H 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, ^1H NMR and ESR Spectrometry which aims to apply this knowledge towards research.
- ✓ Student can understand intrepetaion of NMR and how to structural elucidation.
- ✓ Student can understand the applicatons of ESR spectra.
- ✓ Student can understand to solve the problems of individual spectral methods of UV-IR & PMR.



Prof. M. SUBBARAO
M.Sc., M.Phil., Ph.D.,
Chairman, BOS in Chemistry (PG)
Acharya Nagarjuna University
N.Nagar, Guntur-522 510. A.P. India.

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DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-II: ORGANIC SYNTHESIS & REACTION MECHANISMS-I (R22OC32)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

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, Sandmeyer 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 diacetate and TI(III) nitrate, Lead tetra acetate, SeO₂, MnO₂ Ag₂CO₃, peracids.

Oxidation of C=C perhydroxylation using KMnO₄, OsO₄, 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 borohydrides-Reduction with diimide.

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 Moschr.
- 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.
- ✓ Students can understand the reduction by dissolving metals, reduction with metal and acid.
- ✓ Students can understand the terminology, selectivity in synthesis and analytical methods.



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DEPARTMENT OF CHEMISTRY

M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-III (Elective-A): ALKALOIDS, TERPENOIDS, QUINONES & PHENOTHIAZINES
(R22OC33A)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

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.
- ✓ To learn the about the stereochemistry of alkaloids.

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, ergotamine.
- b) Structure, stereochemistry, synthesis and biosynthesis of Ephedrine, Conine and nicotine.

UNIT-IV

10H

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

Quinones and Phenothiazines:

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

Phenothiazines: Classification, pharmacological properties of phenothiazines, 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.
- 4) Chemistry and physiology of alkaloids by Manske Vol. I & II, VII.
- 5) Medicinal Chemistry by A. Burger.
- 6) Isoquinoline Alkaloids by M. Shamma.
- 7) Heterocyclic Chemistry by J.A. Joule et al., 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.
- ✓ Students can understand the stereochemistry of alkaloids.



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ACHARYA NAGARJUNA UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III
PAPER-III (Elective-B): CHEMISTRY OF AEROSPACE MATERIALS (R22OC33B)
(For the students admitted from the A.Y. 2022-2023 onwards)
Max. Marks: 100 **(Internal-30M & External-70M)**

SYLLABUS

Learning Objectives:

- ✓ To introduce the students to various classes of materials used in aerospace.
- ✓ To understand the materials used and their property requirements for different parts of spacecraft.
- ✓ To study composition- structure-processing-property correlation in aerospace materials to enable them to design new materials with improved property.
- ✓ To understand the metallic materials for cryogenic applications.
- ✓ To study the evaluation of materials for space environment and space worthiness.

UNIT-I **14H**
Carbon Based Materials: Carbon fiber, carbon-carbon composites, carbon aerogels and foams,
Ceramic Materials: Polymer derived ceramics- synthesis, processing of pre-ceramic polymers, ceramic fibers, Ceramic matrix composites, Thermal barrier coatings, Ablative materials, Silica tiles, Ceramic aerogels, Porous ceramics and ceramic foams, Ultrahigh temperature ceramics- TiB_2 , ZrB_2 , HfB_2 and their composites, Materials with zero thermal expansion-glass ceramics- preparation and application.

UNIT-II **12H**
Metallic Materials: Super alloys, Titanium alloys, Intermetallics and metal matrix composites, Functionally graded materials -production, properties and application.

UNIT-III **10H**
High Temperature Polymers: Aromatic liquid crystalline polyesters, Phenolics, Polyimide, Poly ether ether ketones- synthesis, processing and applications.

UNIT-IV **12H**
Materials for Cryogenic Applications: Metals for low temperature applications, Austenitic stainless steel, Nitrogen containing steel, Aluminium, Aluminium-lithium alloys, Titanium alloys, Cryo insulation materials, Polymers and adhesive for cryo temperature applications.

Materials for Space Environment: Radiation shielding materials, Atomic oxygen resistant materials, Space suit materials and materials for life support systems, Evaluation of materials for space environment and space worthiness.

Reference Books:

- 1) G. Savage, Carbon-Carbon Composites, 1st ed., Chapman and Hall, 1993.
- 2) M. Scheffler, P. Colombo, Cellular Ceramics, Structure, Manufacturing, properties and Applications, 1st ed., Wiley-VCH, 2006.
- 3) W.D. Kingery, H.K. Bowen, D.R. Uhlmann, Introduction to Ceramics, 2nd ed., WileyInterscience, 1976.
- 4) J.S. Reed, Principles of Ceramic Processing, 2nd ed., Wiley-Interscience, 1995.
- 5) H.M. Flower, High Performance Materials in Aerospace, 1st ed., Chapman & Hall, 1995.
- 6) B.Horst, B. Ilschner, K.C. Russel, Advanced Aerospace Materials, Springer-Verlag, Berlin, 1992.
- 7) F. Mohammad, Speciality Polymers: Materials and Applications, I.K. International publishing House Pvt. Ltd, 2007.
- 8) W. Krenkel, R. Naslain, H. Schneider, (Eds.) High Temperature Ceramic Matrix composites, 1st ed., Wiley-VCH, 2006.8 13
- 9) T.W. Clyne, P.J. Withers, E.A. Davis, I.M. Ward, Introduction to Metal Matrix Composites, Cambridge Solid State Science Series, 1st ed., Cambridge University Press, 1993.
- 10) R.R. Luise, Applications of High Temperature Polymers, CRC press, 1st ed., 1996.

Learning Outcomes:

- ✓ Students will get introduced to different classes of aerospace materials.
- ✓ Students understands property requirements of materials used in different areas of a spacecraft.
- ✓ Students will get an insight into composition-structure-processing-property correlation of aerospace materials to enable them to design new materials with improved properties.
- ✓ Studetns can understand the metallic materials for cryogenic applications.
- ✓ Studetns can understand the evaluation of materials for space environment and space worthiness.



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DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-III (Elective-C): DRUG DISCOVERY, DESIGN AND DEVELOPMENT (R22OC33C)
(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

Learning Objectives:

- ✓ To learn about the definition of basic principles of pharmacology.
- ✓ To know the discovery of optimization of existing drugs as leads.
- ✓ To know the structure activity / relationship in various drugs.
- ✓ To know the introduction of QSAR & properties.
- ✓ To learn about the structure, uses & mechanisms of action of common drugs.

UNIT-I: Basic Principles of Pharmacology

14 H

Definitions: Disease, drug, bioassay, pharmacokinetics and pharmacodynamics, stages involved in drug discovery, formulation, drug dosing, routes of drug administration,

Pharmacokinetics: Absorption, distribution, metabolism and excretion of drugs (ADME), drug delivery.

Pharmacodynamics: Nature of drug - receptor interactions, theories of drug action: occupancy theory, rate theory, induced-fit theory, macromolecular perturbation theory.

Drug synergism and antagonism, drug toxicity, clinical trials.

UNIT-II: Lead Discovery and Optimization

14 H

Lead Discovery: Existing drugs as leads (me too drugs), pharmacophore. Principles of design of agonists e.g. salbutamol, antagonists e.g. cimetidine and enzyme inhibitors e.g. captopril. Drug discovery without lead. Serendipity-penicillin and librium as examples.

Lead Optimization: Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead, conformational blockers, discovery of oxamniquine.

UNIT-III: SAR

10H

Structure Activity Relationship (SAR): SAR in sulfa drugs, benzodiazepines, and taxol analogs, principles of prodrug design.

UNIT-IV: QSAR Studies

10H

Quantitative Structure Activity relationship (QSAR): Introduction to QSAR, physicochemical properties. lipophilicity: partition coefficient (P) and the lipophilicity substituent constant (π), electronic effects: Hammett constant (σ), steric effects: Taft's constant (Es), Hansch analysis, Craig's plot, Topliss scheme, free Wilson approach, Lipinski rule of five.

UNIT-V: Common Drugs

12 H

Structure, uses, mechanism of action of antibacterial agents: sulfamethoxazole, penicillin G, antiviral agents: acyclovir, indinavir, anticancer agents: mechlorethamine, methotrexate, antifungal agents: fluconazole, griseofulvin, gastrointestinal agents: ranitidine, omeprazole, metoclopramide, cardiovascular agents: amrinone, procainamide, captopril, propranolol, methyl dopa, anticoagulants: warfarin, central nervous system agents: paracetamol, betamethasone, chlorpromazine, levodopa, diazepam, phenytoin, procaine.

Reference Books:

- 1) Medicinal Chemistry and Pharmaceutical Chemistry, H. Singh and Kaur.
- 2) An Introduction to Medicinal Chemistry, 4th Ed., G. L. Patrik.
- 3) Fundamentals of Medicinal Chemistry, Gareth Thomas.
- 4) Biochemical Approach to Medicinal Chemistry, Thomas Nogrady.
- 5) Principles of Medicinal Chemistry, William Foye.
- 6) Medicinal Chemistry, Ashutosh Kar.
- 7) Medicinal Chemistry, R. R. Nadendla.
- 8) Berger's Medicinal Chemistry, Vols. 1-5, Manfred E. Wolf.

Learning Outcomes:

- ✓ Students can understand the pharmacokinetics & pharmacodynamics.
- ✓ Students understand the lead discovery and lead optimization of various existing drugs.
- ✓ Students understand the structure-activity relationship in sulpha drugs, benzodiazepines and principles of prodrug design.
- ✓ Students understand about the quantitative structure-activity relationship of properties.
- ✓ Students understand the structure, uses, mechanism of action of antibacterial, antifungal, antiviral, anticancer agents and also about anticoagulants and central nervous system agents.



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DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-IV (Elective-A): CHEMISTRY OF NATURAL PRODUCTS (R22OC34A)
(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

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 hormones, and synthesis of some steroidal and non-steroidal hormones.
- ✓ To know about aminoacids, proteins, enzymes, cofactors and prostaglandins.
- ✓ To know about the structures and synthesis of insecticides, Rotenoids and Isobutylamines.

UNIT-I

12H

Flavonoids and Prostaglandins

Flavonoids: Classification, 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 A₁, vitamin E (α , β , γ , δ -tocopherols) and vitamin K

Water soluble Vitamins: Chemistry, Synthesis, and biosynthesis of B₁ 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.
- 8) The terpenoids by Simonsen,
- 9) The steroids by Shoppee,
- 10) 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 hormones, and synthesis of some steroidal and non-steroidal hormones.
- ✓ 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. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-IV (Elective-B): CHEMISTRY OF HIGH ENERGY MATERIALS (R22OC34B)
(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

Learning Objectives:

- ✓ To learn about the definitions of high energy materials.
- ✓ To learn about the basis of energetic materials.
- ✓ To know about the theoretical basis of thermodynamics.
- ✓ To know about the importance of various novel energetic materials.
- ✓ To know the handling & synthesis of energetic materials.

Unit -I

10H

High Energy materials: Introduction, Definitions, Combustion, Deflagration, Detonation, Fire and Combustion, Deflagration and Detonation.

Unit-II

12H

Classification of Energetic Materials: Primary Explosives, High (Secondary) Explosives, Propellant Charges, Rocket Propellants, Chemical Thermal Propulsion (CTP), Pyrotechnics, Detonators, Initiators, Delay Compositions and Heat-Generating Pyrotechnics, Light-Generating Pyrotechnics, Decoy Flares, Smoke Munitions, Near-Infrared (NIR) Compositions.

Unit-III

14H

Detonation, Detonation Velocity and Detonation Pressure,

Thermodynamics: Theoretical Basis, Computational Methods, Thermodynamics, Detonation Parameters, Combustion Parameters, Example: Theoretical Evaluation of New Solid Rocket Propellants 101 4.2.5 Example: EXPLO5 Calculation of the Gun Propellant Properties of Single, Double and Triple Base Propellants.

Unit-IV

12H

Design of Novel Energetic Materials: Classification, Polynitrogen Compounds, High-Nitrogen Compounds, Tetrazole and Dinitramide Chemistry, Tetrazole, Tetrazine and Trinitroethyl Chemistry, Ionic Liquids, Dinitroguanidine Derivatives, Co-Crystallization, Future Energetics.

Synthesis of Energetic Materials: Molecular Building Blocks, Nitration Reactions, Processing, Safe Handling of Energetic Materials in the Laboratory, General, Protective Equipment, Laboratory, Equipment. **Energetic Materials of the Future.**

Reference Books:

- 1) G.Majano, S. Mintova, T.Bein, T.M.Klapotke, Advanced Materials.
- 2) R.M.Doherty, Novel Energetic Materials and Applications.
- 3) H.D.B. Jenkins, Chemical Thermodynamics at a Glance, Black well, Oxford.
- 4) J.P. Agarwal, R.D. Hodgson Organic Chemistry of Explosives.
- 5) Prof. Dr. Thomas Kal Potke Energetic Materials-LMU Munich.
(<https://www.hedm.cup.uni-muenchen.de/personen/professors/klapoetke/index.html>)
- 6) <https://www.uidaho.edu/sci/chem/people/faculty/jshreeve>

Learning Outcomes:

- ✓ Students can able to understand the definitions of high energy materials.
- ✓ Studetns can understand the categorization of energetic materials.
- ✓ Students able to understand theoretical basis of thermodynamics with examples.
- ✓ Students can understand about the design of various novel energetic materials.
- ✓ Students understand the synthesizing the energetic material of their importance in future.



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M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PAPER-IV (Elective-C): APPLICATIONS OF SYNTHETIC PRODUCTS (R22OC34C)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

SYLLABUS

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.
- ✓ To introduce the students biodegradable and Non-biodegradable polymers and their industrial importance.

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. Rodfwel, 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.
- ✓ Students understand the biodegradable and Non-biodegradable polymers and their industrial importance.



Prof. M. SUBBARAO
M.Sc., M.Phil., Ph.D.,
Chairman, BOS in Chemistry (PG)
Acharya Nagarjuna University
N.Nagar, Guntur-522 510. A.P. India.

ACHARYA NAGARJUNA UNIVERSITY

DEPARTMENT OF CHEMISTRY

M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III

PRACTICAL-I: MULTISTAGE ORGANIC SYNTHESIS (R22OC35)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

(Minimum Five Experiments must be carryout)

Expt-1: Synthesis of paracetamol 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/paracetamol(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: Phthamide-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 benzophenone 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: Anthranilic acid to *o*-chlorobenzoic acid (Diazotisation 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.

Reference Books:

- 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.Shriener, 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 the Duration is a 9 hours.



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ACHARYA NAGARJUNA UNIVERSITY
DEPARTMENT OF CHEMISTRY
M.Sc. ORGANIC CHEMISTRY :: SEMESTER-III
PRACTICAL-II: ORGANIC ESTIMATIONS (R22OC36)

(For the students admitted from the A.Y. 2022-2023 onwards)

Max. Marks: 100

(Internal-30M & External-70M)

(Minimum Five Experiments must be carryout)

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

Note: For University Practical Examination the Duration is a 6 hours.



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