

SEMESTER-III**BIOORGANIC CHEMISTRY****1. Course Description**

Programme: M.Sc. Organic Chemistry

Max.Hours: 30

Course Code: P24/CHE/GE/301

Hours per week: 2

Course Type: GE

Max. Marks: 50

No. of credits: 2

2. Course Objectives

- To understand the structure and function of DNA & RNA. Biological processes such as DNA replication, Transcription & protein biosynthesis.
- To describe the different synthetic methods of peptides and classification of proteins.
- To study of Enzyme selectivity and its catalytic property in various organic synthetic reactions

3. Course Outcomes

CO1: Discuss the structure and synthesis of nucleosides and nucleotides. Explain primary, secondary and tertiary structure of DNA. Discuss Replication, transcription, translation, genetic code and DNA fingerprinting (**UNDERSTANDING**).

CO2: Explain the Classification, nomenclature and bonding of peptides and biological importance and classification of different structures of proteins. Discuss classification, mechanism of action and factors affecting enzyme catalysis, Enzyme inhibition and immobilized enzymes (**APPLY**).

4. Course Content

MODULE I: NUCLEIC ACIDS

(15 Hrs)

Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of RNA, Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA fingerprinting.

MODULE II: PROTEINS & ENZYMES

(15 Hrs)

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins. Definition. Classification based on mode of action. Mechanism of enzyme catalysis Lock and Key, Induced-Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantioselective – illustration with suitable examples. Factors affecting enzyme catalysis. Enzyme inhibition-reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised

5. References

1. Organic Chemistry by McMurry
2. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
3. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
4. Outlines of Biochemistry by Conn and Stumpf
5. Enzyme structure and mechanism by Fersht and Freeman
6. Enzymes for green organic synthesis by V.K. Ahluwalia
7. Biotransformations in Organic Chemistry by K Faber.
8. Principles of biochemistry by Horton & others.
9. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugasand Christopher Penney.
10. Concepts in Biotechnology by D. Balasubramanian & others

6. Syllabus Focus

a. Relevance to Local, Regional, National and Global Development Needs

Local/Regional/National /Global Development Needs	Relevance
LOCAL	Synthesizing pharmaceutical agents as antiviral agents, antibiotic, prodrug and even antimicrobial agent with proteins and peptides in healthcare
REGIONAL	Gene regulating tools or therapeutic agents for the treatment of human diseases with genetic disorders. Developing sensing platforms for detecting ions, small molecules, proteins, and cells.
NATIONAL	Manufacturing of diverse food products, beverage processing, animal feeding, textile industries, household goods, cleaning products, biofuels and other automotive fuels, and energy generation plants by enzymes.
GLOBAL	High efficient biocatalyst in synthetic organic chemistry in the manufacturing of highly enantiomeric pure stereoisomer in pharmaceutical industry

b. Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Deducing the synthesis of nucleosides and nucleotides for the preparation of DNA & RNA.
EMP	Module No.2	Economically viable solid phase synthetic methods for producing polypeptides
ED	Module No. 3	Practicing organic reactions where enzymes used as oxidizing, reducing, decarboxylase and hydroxylase catalyst to inculcate interest towards pharma industry

2. Pedagogy

S. No	Student Centric Methods Adopted	Type/ Description of Activity
1.	Participative Learning	Presentation
2.	Experiential Learning	Field Trips
3.	Problem solving	Case studies

3. Course Assessment Plan

a. Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA-20M	End Semester Examination-30M
CO1 & CO2	Assignment	Written test

**BIOORGANIC CHEMISTRY
MODEL QUESTION PAPER
THEORY**

Course Code: P24/CHE/GE/301
Credits: 2

Max Marks:30
Max Hours: 1 hrs

SECTION A - INTERNAL CHOICE

Write any 6 out of 8

6Q X 5 M = 30 M

Question Number	Module	Question	CO	BTL
1	Module 1	Explain briefly about the replication and translation of DNA	CO 1	Level II
2	Module 1	Explain briefly about DNA fingerprinting	CO 1	Level II
3	Module 2	Write any two methods of determination of N-terminal amino acid sequence of polypeptides	CO 2	Level I
4	Module 2	Describe the solution phase synthesis of peptides	CO 2	Level II
5	Module 1	Describe secondary structure of DNA	CO 3	Level II
6	Module 2	Write a note on enzyme reversible inhibition	CO 3	Level I
7	Module 1	Illustrate the three synthetic methods of Nucleotides	CO 4	Level II
8	Module 2	Write a note on enzyme immobilization	CO 4	Level I

SEMESTER-III

FORENSIC CHEMISTRY & TOXICOLOGY

1. Course Description

Programme: M.Sc. Organic Chemistry

Max.Hours: 45

Course Code:P24/CHE/DSE/302 Hoursper week: 3

CourseType: DSE-2

Max. Marks: 100

No. of credits: 3

2. Course Objectives

- To introduce about the Forensic chemistry, Qualitative and quantitative forensic analysis of inorganic and organic material.
- To examine petroleum products by various methods, Chemistry of fire and Analysis of trace evidence.
- To explain the principles of Toxicology- Methods of transportation of toxicant

3. Course Outcomes

On completion of the coursethestudent willbe able to:

CO1: Compute absolute entropy from heat capacity data; illustrate the partial molar properties; solve the chemical potential and formulate the Gibbs-Duhem equation.(APPLY)

CO2:Compare the concentration cells, derive the expression forliquid junction potential; analyse electrodepolarization and infer Debye – Huckel – Onsagar equation.(ANALYSIS)

CO3:Assess various operators, choose the postulates and theorems of quantum mechanics; deduce the expression of wave function and energy of particles moving in one- and three-dimensional box. (EVALUATION)

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4. Course Content

MODULE 1: FORENSIC CHEMISTRY-I (15 Hrs)

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methods and instrumental techniques Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

MODULE II: FORENSIC CHEMISTRY-II (15 Hrs)

Examination of petroleum products - Distillation and fractionation - various fractions and their commercial uses - Standard method of analysis of petroleum products – Analysis of petroleum products for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires – Causes of fire - Analysis of arson residues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments, Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

MODULE III: FORENSIC TOXICOLOGY-I (15 Hrs)

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist-Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation of toxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms of poisoning- Toxicological investigation/examination of poisoned death- Interpretation of toxicological data- Courtroom testimony in toxicological cases. Case Histories.





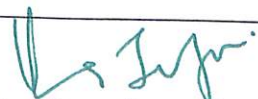
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Recommended books:

1. James, S. H. and Nordby, J. J.: Forensic Science: An Introduction to Scientific and Investigative Techniques, 2003.
2. Saferstein, R: Criminalistics - An Introduction to Forensic Science, Prentice Hall, 1995.
3. Sarkar, S: Fuels and Combustion, Orient Longman, 1990.
4. Verma, R. M: Analytical Chemistry – Theory and Practice, CBS Pub., 1994.
5. Svehla, G. Ed.: Vogel's Qualitative Inorganic Analysis, Longman, 1998.
6. Bassett: Vogel's Text Book of Quantitative Inorganic Analysis, Longman, 1978.
7. Vogel, A. I: Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, ELBS, 1971.
8. Narayanan, T. V: Modern Techniques of Bomb Detection and Disposal, R. A. Security System, 1995.
9. Almirall, J. R. and Furton, K. G: Analysis and Interpretation of Fire Scene Evidence, CRC Press, 2004.
10. Bogusz, M. J: Handbook of Analytical Separations : Vol. 2 ,Forensic Science, Elsevier, 2000.
11. Bureau of Indian Standards: Specifications and Methods of Analysis for Petroleum Products.
12. Wilson and Wilson's Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysis
14. AOAC: Official Methods of Analysis
15. Daeid, N.N.: Fire Investigation: Theory and Practice, Taylor and Francis, 2003
16. Klaassen, C. D.,; Casarett and Doull's Toxicology: The Basic Science of Poisons, 5th ed, McGraw-Hill, 1995.
17. Moffat, A.C. : Osselton, D. M. Widdop, B. : Clarke's Analysis of Drugs and Poisons in Pharmaceuticals, body fluids and postmortem material, 3rd ed., Pharmaceutical Press 2004.

Prepared by	Checked & verified by	Approved by
Name and Signature of the teaching faculty	Name and Signature of HoD	Name and Signature of Principal
 Dr. M. Bhargavi	 Dr. D. Sumalatha	 Dr. Uma Joseph

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SEMESTER-III

GREEN CHEMISTRY AND ORGANIC MATERIALS

1. Course Description

Programme: M.Sc.

Course Code: P24/CHE/DSE/303

Course Type: DSE²

No. of credits: 3

Max.Hours: 45

Hours per week: 3

Max. Marks: 100

2. Course Objectives

- To understand the twelve basic principles of Green chemistry for designing products and processes that minimizes the use and generation of hazardous substances.
- To deal with the carbon nano material's synthesis, Optoelectronic molecules and their applications.
- To impart knowledge of different types of Supramolecules, structures and their applications as organic-inorganic materials and devices.

3. Course Outcomes

CO1: Understand Green Chemistry principles and practices and evaluate sustainable alternatives to traditional chemical processes. **(APPLICATION)**

CO2: Describe the organic nano materials and their applications. **(UNDERSTANDING)**

CO3: Discuss various types of Supra molecules and their application. **(UNDERSTANDING)**

4. Course Content

MODULE I: GREEN CHEMISTRY

(15 Hrs)

PRINCIPLES : Detailed discussion of twelve principles of Green Chemistry with appropriate examples

GREEN SYNTHESIS

- i) Microwave Assisted Organic Synthesis (MAOS):** introduction, benefits and limitations.
- a) Microwave assisted reactions in organic solvents:** Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.
- b) Microwave assisted Solvent-free reactions:** Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.
- ii) Ultrasound Assisted Organic Synthesis:** introduction, applications of ultrasound- Cannizzaro reaction, Reformatsky reaction and Strecker synthesis.
- iii) Organic Synthesis in Green Solvents:** introduction
- a) Aqueous Phase Reactions:** Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and dihydroxylation reactions.
- b) Organic Synthesis using Ionic liquids:** Introduction, applications- Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.
- iv) Green Catalysts in organic synthesis:** introduction
- a) Phase Transfer Catalysts in Organic Synthesis:** Introduction, Williamson ethers synthesis and Wittig reaction
- b) Biocatalysts in Organic Synthesis:** Biochemical (microbial) oxidations and reductions.

MODULE II: ORGANIC NANOMATERIALS

(15 Hrs)

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes. Structures of aromatic belts, nano car and molecular machines

Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)

Natural Benzheterazoles and their synthetic modifications as optoelectronic molecules.

MODULE III: SUPRAMOLECULAR CHEMISTRY

(15 Hrs)

Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation- π , anion- π , π - π and Van der Waals interactions), Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcerands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catenanes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.

Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral framework, Chiral receptor from Kemp's tri acid. Chiral receptors for tartaric acid.

5. References

1. P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker, (2001).
3. M.C. Cann & M.E. Connelly: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers.
6. Enantioselective organocatalysis, Peter I Dalco, Wiley-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
8. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications.
9. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications.
10. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
11. Stereochemistry of organic compounds -Principles & Applications by D Nasipuri
12. Nanochemistry by G.B. Sergeev; Elsevier
13. Nanochemistry: A chemical approach to nano materials , G.A. Ozin & A.C. Arsenault; RSC publishers.

1. Syllabus Focus

a) Relevance to Local, Regional, National and Global Development Needs

Local /Regional/National /Global Development Needs	Relevance
GLOBAL	The study of Organic materials can have a direct impact on local industries and communities by creating job opportunities, fostering innovation, and improving local economies. Local research institutions and universities can also benefit from collaborations and partnerships in this field.
NATIONAL	Green chemistry contributes to achieving sustainability goals, reducing carbon emissions, and increasing energy efficiency. This aligns with national priorities for environmental protection and sustainable development.
LOCAL	Green synthesis can help protect local ecosystems and minimize pollution, ultimately improving the overall quality of life for residents in the area.

b) Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Problem-solving skills in terms of case studies related to environmental issues and pollution prevention.
ED	Module No.2	Research collaborations
EMP	Module No. 3	Encourage critical thinking on research methodologies and applications from publications in journals

2. Pedagogy

S. No	Student Centric Methods Adopted	Type/ Description of Activity
1.	Problem Solving	Case studies
2.	Participative Learning	Presentation
3.	Experiential Learning	Field Trips

3. Course Assessment Plan

a) Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA- 40%	End Semester Examination-60%
CO1	CIA-1 - Written Exam	Written Exam
CO2	CIA-2 – Presentation	
CO3	CIA-2 – Assignment	

b) Model Question Paper-End Semester Exam

**GREEN CHEMISTRY AND ORGANIC MATERIALS
MODEL QUESTION PAPER
THEORY**

Course Code: P24/CHE/DSC/302

Max Marks:60

SECTION A - INTERNAL CHOICE					3Q X 12M = 36 M
Question Number	Module	Question	CO	BTL	
1	Module 1	(a) Define atom economy Explain concept of Atom Economy using different types of Organic Reactions ? (b) What are the advantages and disadvantages of Microwave reactions?	CO 1	Level -II Level -II	
2	Module 1	(a)Discuss the applications of Ultrasound in Canizzaro reaction and Reformatsky reaction. (b) What are ionic liquids ? Give the applications of ionic liquids with reference to Beckmann Rearrangement and Suzuki cross coupling reaction.	CO 1	Level -II Level -II	
3	Module 2	(a)Explain liquid crystal mechanism. (b) Discuss about types of carbon nanotubes and their conductance.	CO 2	Level -II Level -II	
4	Module 2	(a) Account the top down approach in nanochemistry. (b) Discuss about Photochemical devices and molecular muscles.	CO 2	Level -II Level -I	
5	Module 3	(a)Write the various types of supramolecular interactions with examples. (b) Discuss briefly about rotaxanes and catenanes.	CO 3	Level -II Level -II	
6	Module 3	(a)Explain the Enantio selective molecular recognition of cyclodextrins. (b) Discuss about Carcerands and hemicarcerands.	CO 3	Level -II Level -II	
SECTION B - ANSWER ANY 4 OUT OF 6					4Q X 6M = 24 M
(To compulsorily have TWO question from each module)					
7	Module 1	What are the limitations of microwave reactions?	CO 1	Level -II	
8	Module 1	What is PTC? What are the advantages of using PTC in organic reaction?	CO 1	Level -II	
9	Module 2	Write a short note on molecular wire rectifiers.	CO 2	Level -II	
10	Module 2	What are the optoelectronic properties of fullerenes?	CO 2	Level -II	
11	Module 3	What are cryptands and give their uses ?	CO 3	Level -II	
12	Module 3	Write about Enantioselective molecular recognition from Kemp's triacid.	CO 3	Level -II	

a) Model Question Paper-End Semester Exam

**GREEN CHEMISTRY AND ORGANIC MATERIALS
MODEL QUESTION PAPER
THEORY**

TIME: 21/2hrs
Max. Marks: 60

Course Code: P24/CHE/DSE/303

SECTION –A (Essay Questions)

I Answer the following questions

3X12=36 Marks

1. (a) Define atom economy Explain concept of Atom Economy using different types of Organic Reactions ? **(CO1) (Level -II)**
(b) What are the advantages and disadvantages of Microwave reactions? **(CO1) (Level -II)**
OR
2. (a) Discuss the applications of Ultrasound in Cannizzaro reaction and Reformatsky reaction. **(CO1) (Level -II)**
(b) What are ionic liquids ? Give the applications of ionic liquids with reference to Beckmann Rearrangement and Suzuki cross coupling reaction. **(CO1) (Level -II)**
3. (a) Explain liquid crystal mechanism. **(CO2) (Level -II)**
4. (b) Discuss about types of carbon nanotubes and their conductance. **(CO2) (Level -II)**
OR
4. (a) Account the top down approach in nanochemistry. **(CO2) (Level -II)**
(b) Discuss about Photochemical devices and molecular muscles. **(CO2) (Level -II)**
5. (a) Write the various types of supramolecular interactions with examples. **(CO3) (Level -I)**
(b) Discuss briefly about rotaxanes and catenanes. **(CO3) (Level -II)**
OR
6. (a) Explain the Enantio selective molecular recognition of cyclodextrins. **(CO3) (Level -II)**
(b) Discuss about Carcerands and hemicarcerands. **(CO3) (Level -II)**

SECTION –B (Short Answer Questions)

II Answer any four of the following questions

4 X 6 = 24 M

7. What are the limitations of microwave reactions? (CO1) (Level -II)
8. What is PTC? What are the advantages of using PTC in organic reaction? (CO1) (Level -II)
9. Write a short note on molecular wire rectifiers. (CO2) (Level -II)
10. What are the optoelectronic properties of fullerenes? (CO2) (Level -II)
11. What are cryptands and give their uses. (CO3) (Level -II)
12. Write about Enantioselective molecular recognition from Kemp's triacid. (CO3) (Level -II)

b) Question Paper Blue print

Modules	Hours Allotted in the Syllabus	COs Addressed	Section A (No. of Questions)	Total Marks	Section B (No. of Questions)	Total Marks
1	15	1	2	12	2	4×6 = 24
2	15	2	2	12	2	
3	15	3	2	12	2	

2. CO-PO Mapping

CO	PO	Cognitive Level	Class room sessions (hrs)
1	2	Apply	15
2	2	Evaluation	15
3	5	Remember	15

CBCS 2024

SEMESTER-III PRACTICALS

CHEMISTRY LAB: DSE

LAB: SEPARATION OF THREE COMPONENT MIXTURES BY CHEMICAL METHODS AND COLUMN CHROMATOGRAPHY

**Program: M.Sc.
P24/CHE/DSE/302/P
Course: DSE
Semester: III**

**Subject Code:
No. of Hrs. allotted: 4 Hrs / week
No. of Credits : 2**

COURSE OUTCOMES:

CO1: Understand the principle involved in separation of the three component organic mixture based on the solubility.

CO2: Identify various functional groups present in the given organic compound by using a systematic procedure.

CO3: Understand the classical methods of purification and basic principles of Column Chromatography.

Lab course : Separation of three component mixtures by chemical methods and Column Chromatography **4 hrs/week**

Separation of three component mixtures: Separation of three component mixtures by chemical methods. A minimum of four mixtures should be separated and analyzed.

Column Chromatography: Separation of a mixture of 2-Hydroxybenzaldehyde and 3-Hydroxybenzaldehyde, Ortho and para Nitro phenols component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC



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PRACTICAL MODEL PAPER

Course Code: P24/CHE/DSE/302/P
Credits: 2

Max Time:3hrs
Max marks :50 marks

Answer all questions.

Q1. Write the principle involved in the separation of a given Ternary Organic mixture.
10M (CO1)

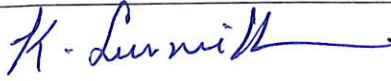




OR


Write the principle involved in the separation of a given Binary Organic mixture by
Column Chromatography(CO3)

Q2. Separate and identify the two components present in the given ternary mixture of
Organic compounds by following a systematic procedure. Submit two derivatives for
each compound and report their melting points. 25M (CO1&CO2)

. Record + Attendance 5M

. Viva 10M

Prepared by Course Teacher [Name & Signature]	Checked &verified by HOD [Name & Signature]	Approved by the Principal
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MODEL PRACTICAL QUESTION PAPER

ISOLATION OF NATURAL PRODUCTS AND THIN LAYER CHROMATOGRAPHY

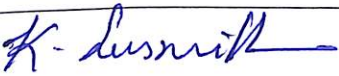



Course Code: P24/CHE/DSE/301/P

TIME: 3hrs


Credits: 2

Max. Marks: 50

1. Write the principle involved in the extraction of caffeine from pepper. **10M (CO1)**
2. a) Separate an unknown binary mixture by TLC and calculate the Rf values.
b) Determination of purity of the compounds/Monitor the progress of a chemical reaction **(25M) (CO2)**
3. Record + Attendance **5M**
4. Viva **10M**

Prepared by Course Teacher [Name & Signature]	Checked & verified by HOD [Name & Signature]	Approved by the Principal
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ISOLATION OF NATURAL PRODUCTS AND THIN LAYER CHROMATOGRAPHY

Program: M.Sc.
Course: DSE-01
Semester: 3

Subject Code P24/CHE/DSE/301/P
No. of Hrs. allotted: 4 Hrs / week
No. of Credits :2

COURSE OUTCOMES

- CO1: Isolation and extraction of Terpenoids & Alkaloids with their medicinal utility in dosage form preparations.
- CO2: Understand the classical methods of purification and basic principles of Thin layer Chromatography.

A. Isolation of the following natural products

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

B. Identification of components in the extracts by TLC


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SEMESTER-III

MODERN ORGANIC SYNTHESIS

1. Course Description

Programme: M.Sc. Organic Chemistry
Course Code: P24/CHE/DSC/302
Course Type: DSC-X
No. of credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 100

2. Course Objectives

- To comprehend stereochemistry and make it possible to synthesize useful chiral molecules with a wide range of scientific applications.
- To support the synthesis of complex organic molecules in a methodical and efficient manner, Retrosynthetic analysis focuses on strategic planning, effective route design, and synthetic pathway optimization.
- To expand synthetic capabilities, improve efficiency and selectivity, address synthetic challenges, and advance fundamental understanding of chemical reactivity. These efforts drive innovation in organic chemistry and have significant implications for drug discovery, materials science, and other fields.

3. Course Outcomes

CO1: Discuss the Prochiral nomenclature Topocity, conditions of stereo selectivity and analytical methods for stereo selective reactions and classification asymmetric synthesis. (UNDERSTANDING)

CO2: Use of various types of synthetic strategies involved in organic synthesis. (APPLICATION)

CO3: Apply a wide range of scientific, technological, and societal impacts, driving innovation and advancement in diverse fields of research and industry. (APPLICATION)

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4. Course Content

MODULE I: ASYMMETRIC SYNTHESIS

(15Hrs)

Introduction: Brief revision of classification of stereo selective reactions Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule.

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphine catalyst.

Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) it's explanation by Zimmerman-Traxel model.

MODULE II: SYNTHETIC STRATEGIES

(15Hrs)

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

Disconnection : Guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials.

Order of events: S-Salbutamol, Propoxycaïne..

One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

Retrosynthesis : Retrosynthesis of Retronecene, Longifoline.

MODULE III: NEW SYNTHETIC REACTIONS, TECHNIQUES AND CONCEPTS IN ORGANIC SYNTHESIS (15Hrs)

- 1. Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck, Stille, Sonogishira cross coupling, and Buchwald-Hartwig coupling reactions.
- 2. C=C Formation Reactions:** Shapiro, Bamford-Stevens, Mc Murrey reactions,
- 3. Multicomponent Reactions:** Ugi, Bergman and Mannich reactions.
- 4. Ring Formation Reactions:** Nazarov cyclisation.
- 5. Click Chemistry:** Click reaction, 1,3-dipolar cycloadditions.
- 6. Metathesis:** Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.
- 7. Other important synthetic reactions:** Baylis-Hilman reaction, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.
- 8. Tandem synthesis:** Tandem reactions; conjugate addition-aldol reaction, electrocyclic-Diels Alder reaction.
- 9. Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.
- 10. Chiron approach in organic synthesis:** Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose.

5. References

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey Aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Named reactions by Jie Jac j Li.

1.Syllabus Focus**a) Relevance to Local, Regional, National and Global Development Needs**

Local /Regional/National /Global Development Needs	Relevance
REGIONAL	Asymmetric synthesis is highly relevant in the field of organic chemistry, particularly in the development of new pharmaceuticals, agrochemicals, and materials.
GLOBAL	Synthetic strategies promote innovation, enhancing research capabilities, improving access to essential resources and technologies, and fostering collaboration and partnerships across borders.
NATIONAL	New synthetic reactions, techniques, and concepts in organic synthesis, foster innovation, advancing scientific research, promoting sustainable practices, and contributing to the improvement of human well-being.

b) Components on Skill Development /Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Review the concept of asymmetric synthesis, emphasizing its importance in producing chiral molecules and pharmaceuticals.
ED	Module No.2	Foster collaboration and partnerships across borders.
EMP	Module No. 3	Develop employability skills by challenging students to explore and propose innovative applications of new synthetic reactions.

2.Pedagogy

S. No	Student Centric Methods Adopted	Type / Description of Activity
1.	Problem Solving	Case studies
2.	Experiential Learning	Field Trips
3.	Participative Learning	Presentation/ Seminar



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3.Course Assessment Plan

a) Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA- 40%	EndSemesterExamination-60%
CO1	CIA-1	Written Exam
CO2	CIA-1	
CO3	CIA-2 Presentation	

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MODERN ORGANIC SYNTHESIS

MODEL QUESTION PAPER
THEORY

Course Code: P24/CHE/DSC/302

Max Marks:60

Credits: 3

Max. Hours: 2½ Hrs

SECTION A - INTERNAL CHOICE		3Q X 12M = 36 M		
Question Number	Module	Question	CO	BTL
1	Module 1	(a) Write a brief note on the following techniques in the determination of enantioselectivity. (i) Specific rotation (ii) Chiral Lanthanide shift reagents. (b) Write an account on enantiotopic ligands and faces.	CO 1	Level -I Level -I
2	Module 1	(a) Explain the asymmetric epoxidation by Sharpless procedure with examples. (b) What is chiral reagent controlled asymmetric synthesis. Explain asymmetric reductions using BINAL-H.	CO 1	Level -II Level -II
3	Module 2	(a) Discuss the terms Functional group addition and Chemoselectivity with suitable examples. (b) Explain Robinson annulation with suitable example.	CO 2	Level -II Level -II
4	Module 2	(a) Explain the concept of two group C-X disconnections using 1,2 and 1,3-difunctionalised compounds (b) What is meant by control in carbonyl condensation? Explain taking Oxanamide.	CO 2	Level -II Level -I
5	Module 3	(a) Formulate Baylis -Hilman reaction and its mechanism. (b) Give an account of Shapiro reaction with mechanism. Explain its regioselectivity with respect to unsymmetrical hydrazones.	CO 3	Level -II Level -II

6	Module 3	(a) What is Metathesis? Explain Ring opening and Ring closing metathesis reactions with examples. (b) Explain the mechanism involved in Suzuki reaction.	CO 3	Level -II Level -II
SECTION B - ANSWER ANY 4 OUT OF 6 4Q X 6M = 24 M (To compulsorily have TWO question from each module)				
7	Module 1	Define substrate selectivity, product selectivity with one example each.	CO 1	Level -I
8	Module 1	Explain Cram's cyclic model with examples?	CO 1	Level -II
9	Module 2	Write the retro synthesis and synthesis of Salbutamol.	CO 2	Level -II
10	Module 2	Define strategic bond and discuss the guidelines for the disconnection of C-X bonds using symmetry in disconnection.	CO 2	Level -I
11	Module 3	Explain Mc Murrey reaction.	CO 3	Level -II
12	Module 3	Explain the Click reaction of 1,3-dipolar cycloadditions.	CO 3	Level -II

b) Model Question Paper-End Semester Exam

MODERN ORGANIC SYNTHESIS

MODEL QUESTION PAPER

THEORY

Course Code: P24/CHE/DSC/302

Max Marks:60

Credits: 3

Max Hours:2½hrs

SECTION-A

I Answer the following questions

3X12=36 Marks

- Write a brief note on the following techniques in the determination of enantioselectivity. (CO1) (Level- I)
 - Specific rotation
 - Chiral Lanthanoid shift reagents
 - Write an account on enantiotopic ligands and faces. (CO1) (Level- I)

OR
- Explain the asymmetric epoxidation by Sharpless procedure with examples (CO1) (Level- II)
 - What is chiral reagent controlled asymmetric synthesis. Explain asymmetric reductions using BINAL-H (CO1) (Level- II)
- Discuss the terms Functional group addition and Chemoselectivity with suitable examples. (CO2) (Level- II)
 - Explain Robinson annulation with suitable example. (CO2) (Level- II)

OR
- Explain the concept of two group C-X disconnections using 1,2 and 1,3-difunctionalised compounds(CO2) (Level- II)
 - What is meant by control in carbonyl condensation? Explain taking Oxanamide (CO2) (Level- II)
- Formulate Baylis –Hilman reaction and its mechanism (CO3) (Level- I)
 - Give an account of Shapiro reaction with mechanism. Explain its regioselectivity with respect to unsymmetrical hydrazones(CO3) (Level- II)

OR
- What is Metathesis? Explain Ring opening and Ring closing metathesis reactions with examples (CO3) (Level- II)
 - Explain the mechanism involved in Suzuki reaction. (CO3) (Level- II)

SECTION-B

II Answer any four questions

4 X 6 = 24 Marks

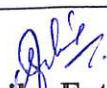




7. Define substrate selectivity, product selectivity with one example each. (CO1) (Level- I)
8. Explain cram's cyclic model with examples? (CO1) (Level- II)
9. Write the retro synthesis and synthesis of Salbutamol. (CO2) (Level- II)
10. Define strategic bond and discuss the guidelines for the disconnection of C-X bonds using symmetry in disconnection. (CO2) (Level- I)
11. Explain Mc Murrey reaction (CO3) (Level- II)
12. Explain the Click reaction of 1, 3-dipolar cycloadditions. (CO3) (Level- II)

a) Question Paper Blueprint

Modules	Hours Allotted in the Syllabus	COs Addressed	Section A (No. of Questions)	Total Marks	Section B (No. of Questions)	Total Marks
1	15	1	2	12	2	4 × 6 = 24
2	15	2	2	12	2	
3	15	3	2	12	2	

4. CO-PO Mapping

CO	PO	Cognitive Level	Classroom sessions(hrs)
1	1	Understanding	15
2	5	Analyse	15
3	6	Create	15

Prepared by	Checked & verified by	Approved by
Name and Signature of the teaching faculty	Name and Signature of HoD	Name and Signature of Principal
 Dr. Sabiha Fatima  Dr. M. Bhargavi	 Dr. D. Sumalatha 	 Dr. Uma Joseph

SEMESTER - III**HETEROCYCLIC AND CONFORMATIONAL ANALYSIS OF CYCLIC COMPOUNDS AND ORD****1. Course Description**

Programme: M.Sc

Course Code: P24/CHE/DSE/301

Course Type: DSE –1

No. of credits: 3

Max. Hours: 45

Hours per week: 3

Max. Marks: 100

2. Course Objectives

- To rationalize the nomenclature, synthesis and reactivity of simple and non aromatic three and four membered heterocyclic compounds with single and two hetero atoms
- To Summarise the synthesis, reactivity and aromaticity of five and six membered heterocyclics with two hetero atoms and the study of seven membered heterocyclic compounds.

3. Course Outcomes

On completion of the course the student will be able to:

CO1: Illustrate the structures of important classes of heterocyclic aromatic organic compounds and able to classify simple heterocyclic aromatic compounds as electron deficient or electron rich and explain their reactivity based on these properties (**UNDERSTANDING**).

CO2: Explain on a mechanistic level, reactions and synthesis of important five membered, six membered and large heterocyclic compounds and purines and pteridines (**REMEMBERING**).

CO3: Assess various conformations possible for alicyclic compounds with their energy & stability. Predicts the configurations of chiral compounds by CD-ORD (**APPLY**).

4. Course Content**MODULE I: INTRODUCTION TO HETEROCYCLIC CHEMISTRY AND NON AROMATIC HETEEROCYCLS (15Hrs)**

Introduction to heterocyclic chemistry, importance of heterocyclic compounds and nomenclature (Brief). Synthesis (any 2 synthetic methods) and reactivity of indole, quinoline, carbazole, benzimidazole, benzoxazole, and benzthiazole.

Nonaromatic heterocyclics: Synthesis (any 3 synthetic methods), reactivity, and importance of the following ring systems: Azirines, Aziridines, Oxiranes, Thiiranes, Oxiranes, Thiiranes, Azetidines, Oxetanes, and Thietanes.




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MODULE II: FIVE AND SIX-MEMBERED HETEROCYCLICS, LARGER RING HETEROCYCLES (15 hrs)

Synthesis (any 3 synthetic methods), reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. 1,2,3-triazoles, 1,2,4-oxadiazole, 1,2,3-thiadiazoles, 1,3,5-triazine
Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine

MODULE III: CONFORMATIONAL ANALYSIS OF CYCLIC SYSTEMS & ORD (15Hrs)


Conformational analysis (Cyclic systems)

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, e. Stereo chemistry of decalins. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes (Oxidation, SN2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule.

5. References

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule&K.Mills
4. Principles of Modern Heterocyclic Chemistry, A.Paquette
5. Heterocyclic Chemistry, J.A.Joule& Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky
7. Aromatic character and aromaticity by G.M.Badger
8. Non-benzenoid aromatic compounds by D.Ginsberg
9. Nonbenzenoid compounds by Lloy
10. Textbook of organic chemistry, Vol II by I L Finar
11. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
12. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
13. Stereochemistry: Conformation & Mechanism by P S Kalsi
14. The third dimension in organic chemistry, by Alan Bassendale
15. Stereo selectivity in organic synthesis by R S Ward.
16. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
17. Optical rotatory dispersion by C Djerassi
18. Optical rotatory dispersion and circular dichroism by P Crabbe
19. Mechanism and Structure in Organic chemistry by S Mukherjee


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6. Syllabus Focus

a) Relevance to Local, Regional, National and Global Development Needs

Local /Regional/National /Global Development Needs	Relevance
Global	Heterocyclic compounds serve as building blocks in the synthesis of pharmaceuticals and fine chemicals in the field of biotechnology.
National	Developing new drugs based on heterocyclic compounds can strengthen a nation's healthcare system by addressing prevalent diseases, reducing mortality rates, and improving public health.
Regional	Heterocyclic compounds are used in the development of agrochemicals, such as pesticides and herbicides. These compounds contribute to increased agricultural productivity, protecting crops from pests and diseases, ensuring food security.
Local	Designing stable and biological molecules in pharma industry through conformational analysis.

b) Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No.1	Practicing the synthesis and reactivity of simple, three & 4 membered heterocyclic compounds
ED	Module No.2	Provide a brief overview of heterocyclic compounds and their diverse applications, emphasizing their significance in pharmaceuticals, agriculture, materials science, and other industries.

EMP	Module No.3	molecular modeling with discussions on real-world applications, promoting both theoretical understanding and practical skills
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7. Pedagogy


S. No	Student Centric Methods Adopted	Type / Description of Activity
1.	Experimental learning	Interactive Classroom Quiz
2.	Preparative learning	Presentation
3.	Problem solving	Case studies

8. Course Assessment Plan

a) Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA - 40%	End Semester Examination-60%
CO1	CIA1-Written Exam	Written Exam
CO2	Skill Test-I – Assignment	
CO3	Skill Test-II – Presentations	


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MODEL QUESTION PAPER
THEORY

Course Code:P24/CHE/DSE/301


Max Marks: 60


Credits :4

Time: 2½Hours

SECTION A - INTERNAL CHOICE			3 Q X 12 M = 36 M	
Question Number	Module	Question	CO	BTL
1	Module 1	(a) Outline the synthesis of carbazole ring system (b) Describe the reactivity of Oxetanes.	CO 1	Level-II Level-II
2	Module 1	(a) Illustrate the reactivity of Azetidines. (b) Outline the synthesis of Thiiranes	CO 1	Level-II Level-II
3	Module 2	(a) Explain electrophilic and nucleophilic substitution reactions of imidazole. (b) Outline the synthesis of pyridazine	CO 2	Level-II Level-II
4	Module 2	(a) Discuss the reactivity of 1,3,5 Triazine. (b) Discuss the synthesis of Caffeine	CO 2	Level-II Level-II
5	Module 3	(a) Discuss the stereochemistry of addition to the carbonyl group in a rigid cyclohexanone. (b) Discuss the stereochemistry of Decalin	CO 3	Level-II Level-II

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CBCS 2024 HETEROCYCLIC & CONFORMATIONAL ANALYSIS OF CYCLIC COMPOUNDS & CD-ORD

6	Module 3	(a) Explain Cotton effect	CO 3	Level-II
		(b) Explain Octant rule with suitable examples		Level-II
SECTION B - ANSWER ANY 4 OUT OF 6		4Q X 6 M = 24 M		
(To compulsorily have Two question from each module)				
7	Module 1	Discuss the fragmentation reactions undergo by aziridines.	CO 1	Level-II
8	Module 1	Give an overview of the Quinoline synthesis	CO 1	Level-I
9	Module 2	Discuss the aromaticity and synthesis of isoxazole.	CO 2	Level-II
10	Module 2	Explain the reactivity of pyrimidine	CO 2	Level-II
11	Module 3	What is 2-alkyl ketone effect?	CO 3	Level-I
12	Module 3	Explain the application of CD curves to study the absolute configuration and conformation of organic molecules with examples	CO3	Level-II

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HETEROCYCLIC AND CONFORMATIONAL ANALYSIS OF CYCLIC COMPOUNDS AND CD –ORD**MODEL QUESTION PAPER
THEORY**

Course Code: P24/CHE/DSE/301
Credits :4

Max Marks: 60
Time: 2½ Hrs

SECTION –A (Essay Questions)**I. Answer the following****4 x 10 = 40 M**

- 1.(a) Outline the synthesis of carbazole ring system. (CO1) (Level 2)
(b) Describe the reactivity of Oxetanes. (CO1) (Level 1)
OR
2. (a) Illustrate the reactivity of Azetidines. (CO1) (Level 2)
(b) Outline the synthesis of Thiiranes. (CO1) (Level 2)
3. (a) Explain electrophilic and nucleophilic substitution reactions of imidazole. (CO2) (Level 2)
(b) Outline the synthesis of pyridazine. (CO2) (Level 2)
OR
4. (a) Discuss the reactivity of 1,3,5 Triazine. (CO2) (Level 2)
(b) Discuss the synthesis of Caffeine. (CO2)
5. (a) Discuss the stereochemistry of addition to the carbonyl group in a rigid cyclohexanone. (CO3) (Level-1)
(b) Discuss the stereochemistry of Decalin. (CO3) (Level-1)
OR
6. (a) Explain Cotton effect (CO3) (Level-2)
(b) Explain Octant rule with suitable examples (CO3) (Level-2)

SECTION –B**Answer any FOUR****4 x 6 = 24 M**

7. Discuss the fragmentation reactions undergo by aziridines. (CO1) (Level-1)
8. Outline the synthesis of Quinoline. (CO1) (Level-2)
9. Discuss the aromaticity and synthesis of isoxazole. (CO2) (Level-2)
10. Explain the reactivity of pyrimidine. (CO2) (Level-2)
11. What is 2-alkyl ketone effect? (CO3) (Level 1)
12. Explain the application of CD curves to study the absolute configuration and conformation of organic molecules with examples (CO3) (Level 2)

SEMESTER-III

PESTICIDES

1. Course Description

Programme: M.Sc. Organic Chemistry
Course Code: P20/CHE/DSE/304
Course Type: DSE -4
No. of credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 100

2. Course Objectives

- To discuss the classification and importance of pesticides. Introduction to Pest control, Biological pheromones, insect juvenile hormones and Environmental pollution from pesticides.
- To differentiate synthetic methods of pesticides, mode of action, formulation and residue analysis of various insecticides.
- To synthesis and give the importance of Insecticides of palnt origin. Concept of Bioinsecticides and pro-insecticides. Synthesis, applications and mode of action of Herbicides

3. Course Outcomes

- CO1: Know the importance, classification of pesticides and how pesticides lead to environmental pollution (**UNDERSTANDING**)
- CO2: Sketch the different synthetic methods and outline the mode of action of pesticides (**REMEBERING**).
- CO3: Outline the synthesis, applications and mode of action of Bio insecticides, pro-insecticides and Herbicides (**EVALUATION**).

1. Course Content

MODULE 1: INTRODUCTION TO PESTICIDES**(15 Hrs)**

- i) **Definition**, Classification and importance of pesticides
- ii) **Pest control**: Different methods –chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.
- a) **Biological**–pheromones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalinal and grandiso pheromones, synthetic sex attractants.
- b) Insect juvenile hormones: JH-A, JH-B, Synthesis of juvabione. Structural formula and importance of methopren.
- c) Moulting hormones-structural formulae and mode of action of ecdysones
- d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agriculture. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Ivermectin, piercidins and phytoalexins.
- iii) **Environmental pollution from pesticides** iv) Integrated pest management.
- v) Pesticide formulations: Dusts, Granules, Wettable powders, Emulsions and Aerosols.

MODULE 2: SYNTHETIC INSECTICIDES**(15 Hrs)**

- i) **Organo chlorine insecticides**- synthesis and mode of action of methoxychlor, perthane, Dicofol, Heptachlor, Dieldrin and Endosulfan.
- ii) **Organo phosphorous insecticides** –synthesis and mode of action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.
- iii) **Carbamate insecticides**- synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.
- iv) Formulation and residue analysis of organochlorine, organophosphorous and carbamate insecticides.

MODULE 3: NATURAL INSECTICIDES AND HERBICIDES**(15 Hrs)**

- i) **Insecticides of plant origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol (Antifeedants).
- ii) Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrethrene.
- iii) **Concept of Bioinsecticides** – Bacillus thuringiensis.

iv) **Concept of pro-insecticides**-structure and mode of action of pro-pheremones and pre-pro-insecticides.


v) **Herbicides** – synthesis, applications and mode of action of the following

a) Aryloxyalkyl carboxylic acid derivative: 2,4-D, MCPA, 2,4,5-T and 2,4,5-TP. b) Carbamates-propham and chloropham, c) Urea derivatives – Monouron and diuron, d) Aliphatic acids-Dalapon, TCA, e) Aromatic acids -2,3,6-TBA, Dicamba and Amiben, f) Nitrogen heterocyclic derivatives – Simazine, Atrazine, Amitrole, Maleic hydrazide Diquat and paraquat, g) Phenols-PCP and Dinoseb, h) Benzonitrile compounds

2. References

- 1) Naturally occurring insecticides: M. Jacobson and D.G. Crosby.
Insecticides for future: Jacobson
- 2) Insect juvenile hormone chemistry and action : J.J Mann and M. Beroza
- 3) Polygodial and warburganal. Terpenoid antifeedants part-II rec, Tran, chin 106
- 4) Insect antifeedants : S.V. Iley & P.L. Toogood, chemistry in Britain, Jan 1990 P.31
- 5) Synthesis of Insecticides : Metcalf
- 6) Fungicides-Frear
- 7) Fungicides-Nene
- 8) Residue reviews vol.36 : Melnikov
- 9) Safer insecticides : E. Hodgson Crop protection agents from Nature: Leonard G Copping
Biofertilizers and Bioinsecticides : A.M. Deshmukh
- 10) Insecticides and Fungicides : U Sriramulu.
Organochlorine insecticides : persistent organic pollutants : F. Moriarty
- 11) Herbicides : P.C. Kearney & D.D. Kaufman
- 12) Analytical Method for pesticides : Z. Weig (Vol III)
- 13) Pesticide formulations : Van Valkenburg
- 14) Insecticides : A.S. Tahori
- 15) Herbicides, fungicides, formulation chemistry - A.S. Tahori


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SEMESTER-III

SYNTHETIC REAGENTS, ^{13}C AND 2D NMR

1. Course Description

Programme: M.Sc. Organic Chemistry
 Course Code: P24/CHE/DSC/301
 Course Type: DSC-9
 No. of credits: 3

Max. Hours : 45
 Hours per week: 3
 Max. Marks: 100

2. Course Objectives

- A protecting group or protective group is introduced into a molecule by chemical modification of a functional group to obtain chemoselectivity in a subsequent chemical reaction, Study of organo metallics in the mechanisms of various organic syntheses are emphasised with prediction of stereo- or regio- chemical consequences.
- Synthetic reagents mostly rely upon the selection and implementation of proper reagents, which may be either used under specific or variety of conditions.
- Identification of compounds using ^{13}C NMR and 2D NMR experiments and elucidates the structure of organic compounds.

3. Course Outcomes

- CO1: Discuss the protection of various functional groups like alcohols, 1,2-diols, amines, carbonyls, carboxylic acids to get the desired result. Explain methods of preparation and applications of organometallic reagents like organo lithium, organo copper, organosilicon, organoborane reagents in organic synthesis. Discuss the reagents used in reactions like Carbonyl methylenation, carbene insertion and C-H activation (**UNDERSTANDING**)
- CO2: Discuss different types of reagents used for oxidation reactions Solve the problems related to reduction reactions. (**UNDERSTANDING**)
- CO3: Discuss types of CMR spectra and methods of recording CMR and 2D NMR spectra. Explain the factors affecting chemical shift and CMR and applications of CMR. Solve the problems based on CMR and 2D NMR spectra. (**APPLICATION**)

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4. Course Content

MODULE I: SYNTHETIC REAGENTS I

(15Hrs)

i) **Protecting groups:**

- a) Protection of alcohols by ether, silyl ether, and ester formation
- b) Protection of 1,2diols by acetal, ketal, and carbonate formation.
- c) Protection of amines by benzyloxy carbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups.
- d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung)groups.
- e) Protection of carboxylic acids by ester and ortho ester (OBO)formation.

ii) **Organometallic Reagents:** Preparation and application of the following in organic synthesis:

- 1) Organolithium 2) Organo copper reagents 3) Organoboranes in C-C bond formation 4) Organo silicon reagents: reactions involving β -carbocations and α -carbanions, utility of trimethyl silyl halides, cyanides and triflates.

- iii) Carbonylmethylenation: a) Phosphorous ylide mediated olefination 1) Wittig reaction, 2) Horner-Wordsworth-Emmons reaction. b) Titanium-Carbene mediated olefination 1) Tebbe reagent 2) Petasis reagent 3) Nysted reagent.

MODULE II: SYNTHETIC REAGENTS II

(15Hrs)

i) **Oxidations:**

- a) Oxidation of active C-H functions: DDQ and SeO₂.
- b) Alkenes to diols: Prevost and Woodward oxidation
- c) Alcohol to carbonyls: CrVI oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation
- d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) **Reductions:**

- a) Catalytic hydrogenation: Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction.
- b) Non-metallic reductions: Diimide reduction
- c) Dissolving metal reductions: Birch reduction.
- d) Nucleophilic metal hydrides: LiAlH₄, NaBH₄, and their modifications.
- e) Electrophilic metal hydrides: BH₃, AlH₃ and DIBAL
- f) Use of tri-n-butyl tin hydride: Radical reductions.

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MODULE III: ¹³C NMR AND 2D NMR SPECTROSCOPY

(15Hrs)

i) **¹³C NMR spectroscopy**: Introduction, Types of ¹³C NMR spectra: uncoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. ¹³C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (¹³C, ¹³CJ) and heteronuclear (¹³C, ¹H J and ¹³C, ²HJ) coupling. Applications of ¹³C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ¹³C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.


ii) **2D-NMR spectroscopy**: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (¹H-¹H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (¹H, ¹³C COSY, HMQC), long range ¹H, ¹³C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUAE experiments and their applications.

5. References:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther

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1. Syllabus Focus

5. Relevance to Local, Regional, National and Global Development Needs

Local/Regional/National /Global Development Needs	Relevance
LOCAL	Organometallic Complex with Favourable Properties for Bioimaging and Applicability in Solid-Phase Peptide Synthesis
REGIONAL	Description of redox reactions is critically important for understanding and rational design of materials for electrochemical technologies
NATIONAL	Multidimensional NMR is also witnessing increased use in quantitative and metabolic screening applications.
GLOBAL	2D NMR with applications in a large range of disciplines, from chemistry and physics to biology and medicine. It is widely used as an analytical tool in all chemistry laboratories and industries,

6. Components on Skill Development/Entrepreneurship Development/Employability

SD/ED/EMP	Syllabus Content	Description of Activity
SD	Module No. 1	Solving CSIR related problems
EMP	Module No.2	Present case studies from industries where we can apply synthetic protocol from organometallic chemistry
ED	Module No. 3	Invite entrepreneurs, professionals, or researchers who apply Advanced NMR to share their experiences and insights

2. Pedagogy

S. No	Student Centric Methods Adopted	Type/ Description of Activity
1.	Problem Solving	Case studies
2.	Participative Learning	Presentation
3.	Experiential Learning	Field Trips

3. Course Assessment Plan

a. Weightage of Marks in Continuous Internal Assessments and End Semester Examination

CO	Continuous Internal Assessments CIA- 40%	End Semester Examination-60%
CO1	CIA-1 - Written Exam	Written Exam
CO2	CIA-2 - Presentation	
CO3	CIA-2 - Assignment	

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c) Model Question Paper- End Semester Exam

SYNTHETIC REAGENTS AND ADVANCED NMR

MODEL QUESTION PAPER

THEORY

Course Code: P24/CHE/DSC/301

Max Marks:60


Credits: 3


SECTION A - INTERNAL CHOICE

3Q X 12 M = 36M

Question Number	Module	Question	CO	BTL
1	Module 1	a) Explain the synthetic applications of Gilman's Reagent. b) Illustrate protection of the carbonyl group by acetal, ketal and thioacetal.	CO 1	Level II Level II
2	Module 1	a) Describe the synthetic applications of Petasis reagent b) Give synthetic applications of organoboranes in C-C bond formation	CO 1	Level II Level I
3	Module 2	(a) Give a note on oxidation using SeO_2 (b) Explain the reduction of aromatic hydrocarbons using Birch reduction and explain the regioselectivity	CO 2	Level I Level II
4	Module 2	a) Compare Woodward and Prevost oxidations. b) Outline the mechanism involved in homogeneous hydrogenation using Wilkinson's catalyst	CO 2	Level IV Level II

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5	Module 3	5.a) How do you calculate the ^{13}C chemical shifts of Alkanes, Alkenes and Alkynes with suitable examples? b) What is an APT spectrum? Explain with suitable example.	CO 3	Level I Level I
6	Module 3	6.a) What is Hetero COSY? Explain the spectrum and its use with one example. b) What are NOESY and 2D-INADEQUATE experiments? Outline their applications giving examples.	CO 3	Level I Level I
SECTION B - ANSWER ANY 4 OUT OF 6 4Q X 6M = 24 M (To compulsorily have Two question from each module)				
7	Module 1	Illustrate the use of Fmoc and CBZ as protecting groups.	CO 1	Level II
8	Module 1	Outline on the mechanism involved in the Wittig reaction.	CO 1	Level II
9	Module 2	Illustrate a brief note on reductions using AlH_3	CO2	Level II
10	Module 2	Explain the oxidative cleavage of 1,2 diols by periodic acid	CO 2	Level II
11	Module 3	Give the applications of DEPT by taking two examples?	CO 3	Level I
12	Module 3	Construct the HOMO-COSY spectrum of ethylchloride.	CO 3	Level VI

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**MODEL QUESTION PAPER
THEORY**

Course Code: P24/CHE/DSC/301/P
Credits: 3

Max Marks:60
Max Hours: 2^{1/2} hrs

SECTION-A

I Answer the following questions

3X12=36 Marks

1. (a) Explain the synthetic applications of Gilman's Reagent. (CO1) (Level II)
(b) Discuss about protection of carbonyl group by acetal, ketal and thioacetal. (CO1) (Level I)

OR

2. (c) Describe the synthetic applications of Petasis reagent (CO1) (Level II)
(d) Give synthetic applications of organo boranes in C-C bond formation (CO1) (Level II)

3. (a) Write a note on oxidation using SeO_2 (CO2) (Level II)
(b) Explain the reduction of aromatic hydrocarbons using Birch reduction and explain the regioselectivity (CO2) (Level II)

OR

4. (c) Compare Woodward and Prevost oxidations. (CO2) (Level II)
(d) Discuss the mechanism involved in homogeneous hydrogenation using Wilkinson's Catalyst (CO2) (Level II)

5. (a) How do you calculate the ^{13}C chemical shifts of Alkanes and Alkenes? (CO3) (Level I)
(b) What is an APT spectrum? Explain with suitable example. (CO3) (Level II)

OR

6. (c) What is Hetero COSY? Explain the spectrum and its use with one example. (CO3) (Level I)
(d) What are NOESY and 2D-INADEQUATE experiments? Outline their applications giving examples. (CO3) (Level II)

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SECTION-B

II Answer any four questions

4 X 6 = 24 M

7. Illustrate the use of Fmoc and CBZ as protecting groups (CO1) (Level I)
8. Write a brief note on the mechanism involved in Wittig reaction. (CO1) (Level II)
9. Write a brief note on reductions using AlH₃ (CO2) (Level II)
10. Explain the oxidative cleavage of 1,2 diols by periodic acid (CO2) (Level I)
11. Give the applications of DEPT by taking two examples? (CO3) (Level I)
12. Draw the HOMO-COSY spectrum of ethylchloride. (CO3) (Level V)

b. Question Paper Blueprint

Modules	Hours Allotted in the Syllabus	COs Addressed	Section A (No. of Questions)	Total Marks	Section B (No. of Questions)	Total Marks
1	15	1	2	12	2	4 × 6 = 24
2	15	2	2	12	2	
3	15	3	2	12	2	

4. CO-PO Mapping

CO	PO	Cognitive Level	Classroom sessions (hrs)
1	1	Application	15
2	2	Evaluation	15
3	2	Evaluation	15

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SEMESTER III

PRACTICALS

CHEMISTRY LAB: DSC- 9

LAB: Synthesis of Organic molecules

Program: M.Sc.
Course: DSC-9
Semester: 3

Subject Code P20/CHE/DSC/301/P
No. of Hrs. allotted: 4 Hrs / week
No. of Credits : 2

PAPER-I SYNTHESIS OF ORGANIC MOLECULES


COURSE OUTCOMES:


- CO1. Will be acquire the skill and acquainted with the knowledge of single and multi step organic preparations.
- CO 2. Understand distillation techniques for purification of organic compounds.
- CO3. Determine the purity of the synthesized compounds and monitor the progress of a chemical reactions involved in synthesis of organic molecules.

Paper-I Synthesis of Organic molecules

- ✓ 2-Phenyl Indole (Fischer indole synthesis), 2,5-Dihydroxy acetophenone (Fries reaction), 4-Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from Benzoin (Benzilic acid rearrangement), Benzpinacol (Photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of Maleic anhydride, Benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from Vanillin (NaBH₄ reduction), 2- and 4-Nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

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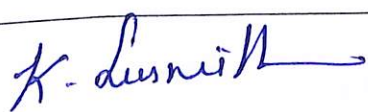
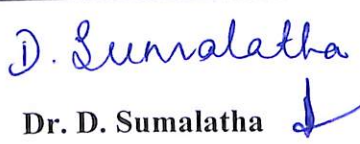


PRACTICAL MODEL PAPER

Course Code: P24/CHE/DSC/301/P
Credits: 2

Max Time:3hrs
Max marks :50 marks


Answer all questions.

- Q1. Write the principle involved in the preparation of the given Organic compound. 10M (CO1)
- Q2. Synthesize the given organic compound by following systematic procedure and check the purity of the compound by TLC. (25M) (CO2 &CO3)
- Q3. Record + Attendance 5M
- Q4. Viva 10M (CO1, CO2 &CO3)

Prepared by	Checked & verified by	Approved by
Name and Signature of the teaching faculty	Name and Signature of HoD	Name and Signature of Principal
 Dr. K.Susmitha	 Dr. D. Sumalatha	 Dr. Uma Joseph
 Dr. Sabiha Fatima		

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