SEMESTER –III

GREEN CHEMISTRY AND ORGANIC MATERIALS

THEORY

Programme: M.Sc. **Max. Hours: 60**
Course Code: P20/CHE/DSE/303 **Hours Per Week: 4**
Course Type: DSE-3 **Max. Marks: 100**
No. Of Credits: 4

COURSEOBJECTIVES

1. Green chemistry focuses on the twelve basic principles of Green chemistry for designing products and processes that minimize the use and generation of hazardous substances.
3. This module elaborates organic synthesis by Microwave, ultra sound, green solvent and catalyst in organic synthesis as alternative methods to conventional methods.
4. To deal with the carbon nano material's synthesis, Optoelectronic molecules and their applications.
5. To impart knowledge of different types of supramolecules, structures and their applications as organic-inorganic materials and devices.

COURSE OUTCOMES

CO1: Discuss a green synthesis using principles of prevention of waste/by-products/toxic products, atom economy.
CO2: Design safer chemicals, selection of appropriate auxiliaries, use of catalytic reagents, prevention of chemical accidents and development of analytical techniques.
CO3: Explain Microwave assisted reactions in organic solvents and solvent free reactions, ultra sound assisted organic synthesis.
CO4: Discuss Organic synthesis in aqueous phase and ionic liquids. Explain Phase transfer catalyst and biocatalyst in organic synthesis.
CO5: Acquire the knowledge of organic nano materials, approach & nanomanipulation.
CO6: Discus the applications of carbon nano: nano car & molecular machines. Discuss the Synthetic modifications of natural products as Opto electronic molecules
CO7: Discuss and explain lock & key model of various structures such as cryptand
CO8: Explain Enantioselective molecular recognition of cychiral receptors.

MODULE1: PRINCIPLES OF GREEN CHEMISTRY

Green chemistry: Introduction

(15 Hrs)

Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals ; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization – careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

MODULE 2: GREEN SYNTHESIS (15 Hrs)

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-Cannizaro 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 diydroxylation 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 ether synthesis and Wittig reaction
b) **Biocatalysts in Organic Synthesis:** Biochemical (microbial) oxidations and reductions.

MODULE 3: ORGANIC NANOMATERIALS (15Hrs)

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, Armchairand Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (ZigZag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes. Structures of aromatics belts, nano car and mmechanism and structures) Natural Benzheterazoles and their synthetic modifications as

optoelectronic molecules.

Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures) Natural Benzheterazoles and their synthetic modifications as optoelectronic molecules.

MODULE 4: SUPRAMOLECULAR CHEMISTRY

I**ntroduction**: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions), Ionophore and molecular receptors.

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

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, 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 triacid .Chiral receptors for tartaric acid

Recommended books:

1. P.T. Anastes& J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
M.C. Cann& M.E. Connely: Real-World cases in Gre

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MODEL THEORY QUESTION PAPER

Course Code: P20/CHE/DSE/303 **Max. Time:21/2hrs**
Credits:4 **Max Marks: 60**

SECTION-A

Answer All Questions **4 x 10=40M**

1 a) Define atom economy Explain concept of Atom Economy using different types of Organic Reactions ? **(CO1)**
b) Write a short note on Green Solvents,(CO2)

OR

2. a) Prevention of hazardous materials **(CO2)**
b) Disadvantages of derivetization**(CO2)**

3. a) What are the advantages and disadvantages of Microwave reactions? **(CO3)**
b) Discuss briefly about microwave assisted solvent free reaction. **(CO3)**

OR

4. a) What are ionic liquids ? Give the applications of ionic liquids with reference to Beckmann Rearrangement and Suzuki cross coupling reaction.**(CO4)**
b) Discuss the applications of Ultrasound inCanizzaro reaction and Reformatsky reaction.**(CO4)**

5. a)Explain liquid crystal mechanism**. (CO7)**
b) Discuss about types of carbon nanotubes and their conductance**. (CO6)**

OR

6. a)Account the top down approach in Nanochemistry**. (CO5)**
b) Discuss about Photochemical devices and molecularmuscles **. (CO6)**

7. a) Write the various types of supramolecular interactions with examples**. (CO7)**
b) Discuss briefly about rotaxanes and catenanes**. (CO7)**

OR

8. a) Explain the Enantio selective molecular recognition of cyclodextrins. **(CO8)**
b) Discuss about Carcerands and hemicarcerands. **(CO7)**

SECTION-B

II Answer any <u>FIVE</u> **5 x 4 =20 M**

9. What are the advantages of aqueous reaction? **(CO1)**
10. Give an account on Solvent free reactions. **(CO2)**
11. What are the limitations of microwave reactions? **(CO3)**
12. What is PTC? What are the advantages of using PTC in organic reaction? **(CO4)**
13. Write a short note on molecular wire rectifiers. **(CO5)**
14. What are the optoelectronic properties of fullerenes? **(CO6)**
15. What are cryptands and give their uses**. (CO7)**
16. Write about Enantioselective molecular recognition from Kemp's triacid. **(CO8)**