

## Ph. D Course Work

Semester I				
Serial Number	Subject Code	Subject	Contact Hours Per Week (L+T+P)	Credits
1		Paper I: Research methodology: Paper writing, thesis writing, ethics & plagiarism		2
2		Paper II: Research & Publication Ethics		2
4		Paper III: Instrumental techniques for characterization of materials		4
5		Paper IV: Elective(s) Reactions and Reagents in Organic Synthesis Multicomponent Reactions in Drug Discovery Green methods in organic synthesis NHC Carbene in organic synthesis Methodologies in asymmetric synthesis Polymer Chemistry		4
		Paper V: Elective(s) Supramolecular Chemistry & Applications Modern Bio-inorganic chemistry Water pollution and its remediation Introduction to Material chemistry and catalysis		4
<b>Total Credits</b>				<b>16</b>

## **Semester I**

### **RESEARCH METHODOLOGY**

#### **UNIT-I**

Definition and purpose of research, types of research, research approaches, research hypothesis, process of designing and doing a research project.

#### **UNIT-II**

Carrying out literature review, introduction to chemical abstracts, SciFinder, Beilstein database, various sources of online articles and papers for browsing and downloading.

#### **UNIT-II**

Principle, instrumentation, and application of various analytical techniques. Stages of research, Writing dissertation.

#### **BOOK SUGGESTED:**

1. A Hand Book of Methodology of Research – P. rajamal and P. Devadoss, R.M.M.Vidya Press (1976).
2. Kothari, C.R.,1985, Research Methodology- Methods and Techniques, New Delhi, Wiley Eastern Limited.
3. instrumental Methods of Analysis – H.H. Willard, L.L.Merritt, J.a.Dean, F.A. Settle, CBS Publishers & Distributors, 1986.

### **Research & Publication Ethics**

#### **UNIT-I**

Necessary attributes of a research scholar, ethical standards that a researcher should follow, biological and environmental ethics.

#### **Unit II**

Methods of data collection, types of data, types of observation, precision and accuracy, types of error, standard deviation, significant figures, validity and reliability of data.

#### **UNIT-III**

Ethical issues relating to research, writing a research report, writing proposal, use of chemistry software, research presentation.

#### **BOOK SUGGESTED:**

1. A Hand Book of Methodology of Research – P. rajamal and P. Devadoss, R.M.M.Vidya Press (1976).
2. Kothari, C.R.,1985, Research Methodology- Methods and Techniques, New Delhi, Wiley Eastern Limited.
3. instrumental Methods of Analysis – H.H. Willard, L.L.Merritt, J.a.Dean, F.A. Settle, CBS Publishers & Distributors, 1986.

### **Reactions and Reagents in Organic**

## Synthesis Reactions:

Aldol type reaction, Algar-Flynn-Oyamada reaction, Alkyne coupling, Suzuki Coupling, Sonagishara reaction, Balz-Schiemann reaction, Barbier-Wieland Degradation, Barton-Zard Pyrrole Synthesis, Bergman Cyclization, Biginelli Reaction

## Reagents:

Azobisisobutyronitrile, Bis(pyridine)iodonium(I) tetrafluoroborate, Bis(trimethylsilyl)amine, Comins' reagent, 1,5-Diazabicyclo(4.3.0)non-5-ene, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone, Tetrakis(triphenylphosphine)palladium(0)

## References:

1. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, Michael G. Eller, Frank G. Favaloro Jr. Publisher Wiley
2. Named Organic Reactions, Second Edition by Thomas Laue and Andreas Plagens John Wiley & Sons: Chichester, England, New York, 2005
3. Advanced Organic Chemistry: Reaction And Synthesis (Part B) Carey and Sundberg
4. Fieser's Reagents for Organic Synthesis Publisher Wiley
5. Comprehensive organic name reactions and reagents by Zerong Wang

## Multicomponent Reactions in Drug Discovery

### Unit 1.

Basic concept of multicomponent reactions: Introduction and Definitions, Type of multicomponent reactions: three-component approach, four-component approach etc. with examples

Biginelli Reaction, Hantzsch Reaction, Ugi Reaction

### Unit 2.

Synthesis of heterocyclic compounds via multicomponent reactions: five-membered, six-membered, Synthesis of Fused Heterocycles.

### Unit 3.

Multicomponent Reactions Based on Nucleophilic Addition to Imines: Strecker Reaction, Mannich Reaction, Petasis Reaction.

Isocyanide-Based Multicomponent Reactions: Passerini Reaction

## References:

1. Synthesis of Heterocycles Via Multicomponent Reactions I & II, Romano Orru, Romano V. A. Orru, Eelco Ruijter, Springer Publications.
2. Heterocyclic Chemistry in Drug Discovery, Jie Jack Li, Wiley Publications.
3. Weber, L. Multi-component reactions and evolutionary chemistry. *Comb. Chem.* **2002**, 7,143-147.
4. Hulme, C.; Gore, V. Multi-component reactions: Emerging chemistry in drug

discovery. From xylocaine to crixivan. *Curr. Med. Chem.* **2003**, *10*, 51-80.

5. Tietze, L. F.; Modi, A. Multicomponent domino reactions for the synthesis of biologically active natural products and drugs. *Med. Res. Rev.* **2000**, *20*, 304-322.

## **Green methods in organic synthesis**

### **Unit 1**

Introduction, Reaction in water: Diels-Alder Reactions, 1,3-Dipolar Cycloadditions, Claisen Rearrangement, Multicomponent reactions, Nucleophilic substitution reactions, Transformations Catalyzed by Transition Metals.

### **Unit 2**

Ionic Liquid: Definition and Introduction, ionic liquid in organic reactions, Ionic Liquids as Solvent, Ionic Liquids as Catalyst.

### **Unit 3**

The Role of Ionic Liquids in Specific Reactions: Cyclocondensation Reactions, Synthesis of Three- Membered Heterocycles, Synthesis of Five-Membered Heterocycles, Synthesis of Six-Membered Heterocycles with some examples.

## **References:**

1. Green Chemistry and Catalysis, R. A. Sheldon, Isabella Arends, Ulf Hanefeld, Wiley Publications.
2. Wasserscheid, P.; Welton, T. *Ionic Liquids in Synthesis*; Wiley-VCH Verlag: Stuttgart, Germany, 2002.
3. Li, C.-J.; Chan, T.-H. *Organic reactions in aqueous media*; Wiley: New York, 1997.
4. *Organic Synthesis in Water*; Grieco, P. A., Ed.; Blackie: London, 1998.
5. Chanda, A.; Fokin, V. V. Organic Synthesis "On Water" *Chem. Rev.* **2009**, *109*, 725-748.

## **NHC Carbene in organic synthesis**

### **Unit 1**

Introduction: Historical background and synthesis of NHCs.

### **Unit 2**

Carbene stability and electronic structure. Structural Versatility: Chelation, Functionalization, immobilization, chirality, ionic liquids.

### **Unit 3**

Selected Catalytic Processes of NHCs: Furan synthesis, hydrogenation, hydroformylation, hydrosilylation, Stille couplings, Sonagashira coupling, Polymerization, aryl amination, olefin metathesis, Kumada coupling, Suzuki coupling, Heck reaction, transesterification.

### **References:**

1. N-Heterocyclic Carbenes in Synthesis Edited by Steven P. Nolan. Wiley-VCH, ISBN : 978 -3 - 52 - 731400 - 3
2. N-Heterocyclic Carbenes by Silvia Díez-González. ISBN: 978-1-84973-042-6 DOI:10.1039/978-1-84-973216-1

## **Methodologies in asymmetric synthesis**

### **Unit 1**

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

### **Unit 2**

Chiral auxiliary controlled asymmetric synthesis:  $\alpha$ -Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in aldol reaction.

### **Unit 3**

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

### **Unit 4**

Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalys. Enzyme mediated enantioselective synthesis

### **References:**

1. Asymmetric synthetic methodology by David J. Ager; CRC Press. ISBN: 978-0-84-938942-9
2. Principles of Asymmetric Synthesis, 2<sup>nd</sup> edition By Robert E. Gawley, Jeffrey Aube;Elsevier. ISBN: 978-0-08-044860-2.

## **Supramolecular Chemistry & Applications**

### **Unit I**

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

### **Unit II**

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complementarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules. Crystal engineering: role of H-bonding and other weak interactions.

### **Unit III**

Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature

### **Unit-IV**

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic, Molecularly imprinted polymers.

### ***Recommended books and References***

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999)
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)
4. Supramolecular Chemistry, Jonathan W. Steed, Jerry L. Atwood, John Wiley & Sons, 09-Jan-2009
5. Supramolecular Chemistry - Fundamentals and Applications, **Ariga**, Katsuhiko, **Kunitake**, Toyoki, Springer
6. Applications of Supramolecular Chemistry, Hans-Jörg Schneider, CRC Press, Taylor & Francis Group
7. Supramolecular chemistry: an introduction, Fritz Vögtle, F. Alfter, Willey
8. Principles and methods in supramolecular chemistry, Hans-Jörg Schneider, Anatoly K. Yatsimirsky, J Willey
9. Introduction to Supramolecular Chemistry, Helena Dodziuk, Springer
10. Self-assembly in Supramolecular Systems, Leonard F. Lindoy, Ian M. Atkinson, RSC

