ST. JOSEPH'S COLLEGE (AUTONOMOUS)

BENGALURU - 27

DEPARTMENT OF CHEMISTRY

SYLLABUS FOR POSTGRADUATE COURSE
M.Sc. ANALYTICAL / ORGANIC CHEMISTRY
FOURTH SEMESTER - DEPARTMENT ELECTIVE

2021-2024

Re-accredited with 'A++' GRADE and 3.79/4 CGPA by NAAC
Recognised as "College of Excellence" by UGC

FROM 2021-2022 ONWARDS

Semester	IV
Paper code	CHDE 0521
Paper title	Dept. elective: SUPRAMOLECULAR CHEMISTRY
Number of teaching hours per week	4
Total number of teaching hours per semester	60
Number of credits	4

1. INTRODUCTION TO SUPRAMOLECULAR CHEMISTRY (6 + 2) h

Definition and development of supramolecular chemistry - lock and key analogy, cooperativity-pre-organisation-complementarity-thermodynamic, kinetic selectivity-nature of supramolecular interactions- solvation effects, supramolecular concepts and design. Host-guest chemistry. Synthesis: The template effect and high dilution.

Lariat ethers, podands, cyclodextrins cyclophanes, cryptophanes, carcerands, hemicarcerands.

Anion binding: Concepts in anion host design, different types of anion hosts. Simultaneous cation and anion binding. Cation-binding: crown ethers, cryptands, spherands, calixarenes (review-recall),

2. NATURE OF SUPRAMOLECULAR INTERACTION 3 h

Ion-ion interactions, ion-dipole interaction, dipole-dipole interaction, hydrogen bonds, hydrophobic interactions.

3. CRYSTAL ENGINEERING 10 h

Self-assembling capsules, molecular containers, metal directed capsules, hydrogen bonded capsules, concepts in crystal engineering, The Cambridge structural database, crystal engineering with hydrogen bonds, pi interactions - halogen bonding and other weak interactions, co-crystal, salts, polymorphs and their physico-chemical properties, coordination polymers. Solid state reactivity: metal-organic frameworks, guest properties of metal-organic frameworks.

4. SOLID STATE SUPRAMOLECULAR CHEMISTRY 8 h

Zeolites: structure, composition and catalysis. Clathrates: urea/thiourea clathrates, trimesic acid clathrates, clathrate hydrates (structure and function of the above species), uses. Inclusion compounds, intercalation compounds.

5. SELF-ASSEMBLY 12 h

Self-assembly in synthetic systems: pi-electron donor-acceptor systems, transition metal directed assemblies, hydrogen bond assemblies, anion directed assemblies, catenanes, rotaxanes, helicates, helical assemblies and molecular knots.

Guest binding by cavitands - calixarenes, resorcarenes, glycourils, cyclodexdrins; molecular clefts, tweezers, cyclophanes, cryptophanes, carcerends and hemicarcerends.

Molecular devices: Photo-switchable devices. Applications of supramolecular chemistry in sensors, switches and molecular machinery and molecular biology.

6. BIOLOGICAL MIMICS AND SUPRAMOLECULAR CATALYSIS 3 h

Characteristics of biological models. Supramolecular catalysis: cyclodexdrin as enzyme mimics.

7. SURFACTANTS AND INTERFACIAL ORDERING 3 h

Micelles and vesicles, surface self-assembled monolayers**.** Application to medicinal chemistry**.** Soft lithography, microlens arrays, transfer printing.

8. DENDRIMERS 5 h

Synthesis - divergent and convergent methods, host-guest chemistry of dendrimers. Supramolecular dendrimer assemblies. Applications of dendrimer for drug delivery.

9. NANOMATERIALS WITH SUPRAMOLECULAR STRUCTURE 8 h

Nanorod, nanowire self-Assembly: metal templating nanowires. Self-assembling nanorods. nanorod devices – nanotubes from nano porous templates. VLS synthesis of nanowires, nanowire quantum size effects. Manipulating nanowires, nanowire sensors.

Nanocluster self-assembly: synthesis of metal capped semiconductor nanoclusters, electrons and holes in nanocluster boxes, nanocrystal semiconductor alloys, nanocluster phase transition water soluble nanoclusters. Polymer nanocomposites.

REFERENCES:

1. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley, 2nd Edn., (2009).
2. Core Concepts in supramolecular Chemistry and Nanochemistry, J. W. Steed, T. R. Turner and K. J. Wallace, John Wiley & Sons, (2007).
3. Supramolecular Chemistry, L.-M. Lehn, VCH, 1995.
4. Crystal Design: Structure and Function, G. R. Desiraju (Ed.), John Wiley and Sons, (2003).
5. Supramolecular Chemistry: An Introduction Vögtle, F. John Wiley & Sons (1993).
6. Concepts of Modern Catalysis and Kinetics, I. Chorkendorff, J. W. Niemantsverdriet, Second Edition, Wiley-VCH Publishers, 2007.
7. Supramolecular chemistry (Oxford university press, 1999) P. D. Beer, P A Gale, D. K. Smith.

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Code number and Title of the paper: **CH DE 0521:** Supramolecular Chemistry

Chapter Number	**Title**	**Number of teaching hours (As mentioned in the syllabus)**	**Maximum marks for which questions are to be framed from this chapter (including bonus questions)**
1.	**Introduction to supramolecular chemistry**	8	13
2.	**Nature of Supramolecular Interaction**	3	6
3.	**Crystal Engineering**	10	17
4.	**Solid State Supramolecular Chemistry**	8	12
5.	**Self-Assembly**	12	20
6.	**Biological Mimics and Supramolecular Catalysis**	3	6
7.	**Surfactants and Interfacial Ordering**	3	6
8.	**Dendrimers**	5	10
9.	**Nanomaterials with supramolecular structure**	8	12
Total marks excluding bonus questions			70

Total marks including bonus questions	103