Course No	Course Name	L-T-P-Credits
CY 542	**Supramolecular Chemistry**	**3-0-0: 3**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic foundation to the understanding of non-covalent interactions, host guest systems, crystallization, synthesis of supramolecular architectures and crystal engineering.

Course Outcomes: After successful completion of the course, students will be able to:

1. Understand structures and properties of various supramolecular systems.
2. Understand intermolecular interactions involving various supramolecular systems.
3. Understand the designing and synthesis of supramolecular systems.
4. Understand the solution state behaviour of supramolecules.
5. Understand crystallization, crystal nucleation and growth.
6. Understand the role of intermolecular interactions in molecular packing in crystals lattice from experimental and computational perspectives.
7. Apply the concept of intermolecular interactions to predict supramolecular synthon in crystal forms.

SYLLABUS

Module	Contents	Hours
I	**Introduction** Concept, development and classification, molecular recognition, host, guest and receptor systems. Nature of supramolecular interactions, hydrogen bonding, ionic bonding, π-stacking, van der Waals and hydrophobic interaction. Self-assembly processes in organic systems: Catenanes, rotaxanes, pseudorotaxanes. Synthetic strategies for their preparation.	5
II	**Cation Binding Hosts** Crown ether, cryptand, spherand and podand. Nomenclature, selectivity and solution behaviour. Alkalides, electrides, calixarenes, siderophores.	6
III	**Anion Binding Hosts** Challenges in the design of anion host, tripodal receptors, neutral receptors, calixpyrroles, metal-containing receptors.	6
IV	**Hosts for Neutral Receptors** Clathrates, inclusion compounds, zeolites, intercalates and coordination polymers.	5
V	**Supramolecular Interaction in Life** Ionophores, porphyrin and other related macrocycles, coenzymes, neurotransmitters, DNA, protein folding, and biochemical self-assembly**.**	6

VI	**Crystal Engineering** Crystal nucleation and growth, properties, design and synthesis of molecular solid-state structures, supramolecular synthons in crystal engineering, crystal forms and their applications. Computational approaches for intermolecular interaction energy, lattice energy, crystal structure prediction.	8

Essential Readings:

1. J. W. Steed and J. L. Atwood, "Supramolecular Chemistry", Wiley-Blackwell, 2nd Edition, 2017.
2. J. M. Lehn, "Supramolecular Chemistry: Concepts And Perspectives", Wiley VCH, 1st Edition, 2014.

Supplementary Readings:

1. G. R. Desiraju, J. J. Vittal and A. Ramanan, "Crystal Engineering: A Textbook", World Scientific Publishing Company, 2011.
2. K. Ariga and T. Kunitake, "Supramolecular Chemistry-Fundamentals and Applications: Advanced Textbook", Springer, 1st Edition, 2006.