Subject Code : P8CHE4

SUPRAMOLECULAR CHEMISTRY & CRYSTAL ENGINEERING

UNIT 1

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H…X interactions, Halogen bonds. π – π interactions,non – bonded interactions. Various types of molecular recognition.

Crystal engineering of Organic solids: Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs. Concepts of different types of synthons based on non-covalent interactions. Principles of crystal engineering and non-covalent synthesis. Polymorphism and Pseudopolymorphism. Supramolecular isomorphism / polymorphism. Crystal engineering of pharmaceutical phases.

UNIT II

M.O.F (Metallo Organic Frame works), Organometallic systems. Combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids. Inter ligand hydrogen bonds in metal complexes – implications for drug design. Crystal engineering of NLO materials,OLED.

UNIT III

Corecptor Molecules and Multiple Recognition:
Dinuclear and Ploynulclear Metal ion Cryptates. Linear recognition of molecular length by Ditopic Coreceptors. Heterotopic Coreceptors- Cyclophane Receptors, Amphiphillic Receptors, Large molecular cages. Multiple Recognition in Metalloreceptors. Supramolecular dynamics.

UNIT IV

Supramolecular Reactivity and Catalysis
Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors.Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications.

UNIT V

Supramolecular Devices and Sensors: Various types of supramolecular devices – an overview. Supramolecular Photochemistry: Molecular and Supramolecular Photonic Devices – Light conversion and Energy transfer Devices. Molecular

and Supramolecular Electronic Devices – Electronic conducting Devices - Molecular wires, Modified and Switchable Molecular wires. Molecular and Supramolecular Ionic Devices – Tubular Mesophases, Molecular Protonics. Switching Devices: Photo switching and Electro switching. Ion and molecule sensors. Role of supramolecular chemistry in the development of nanoscience and technology.

References:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids, Elsevier, Amsterdam, 1989.
3. Desiraju, G.R. & Steiner, T. The weak Hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999.
4. Jeffrey, G. A. Introduction to Hydrogen Bonding ; Oxford University press: New York, 1997.
5. Lehn, J.M. Transition metals in supramolecular chemistry : John Wiley & sons: New York, 1999.
6. Desiraju, G.R. (2001). Current Science, 81, 1038.
7. Rao, C.N.R. (2001). Current Science, 81, 1030.
8. "Molecule Matters" Saravanakumar, k & Sankararaman, S, (2007) Resonance,Vol.12, No 11, Page 77.
9. Journals
   (i)Crystal Growth and Design,
   http://www.pubs.acs.org/journals/cgdefu/index.html
   (ii)Crystal Engineering Communication,
   http://www.rsc.org/Publishing/Journals/ce/index.asp