Tutor Marked Assignment

MCHE-013: SUPRAMOLECULAR CHEMISTRY

Course Code: MCHE-013
Assignment Code: MCHE-013/TMA/2026-27
Maximum Marks: 100

Note: Attempt all questions. The marks for each question are indicated against it.

1.	a)	Explain dipole-dipole interactions in supramolecular chemistry with a suitable example. What is its energy range and why are they important? When are they helpful in molecular recognition?	(5)
	b)	Explain the lock and key principle of binding in supramolecular chemistry with suitable diagrams.	(5)
2.	a)	What are the different types of supramolecular complexes? Illustrate your answer.	(5)
	b)	Give the differences between enthalpy-driven and entropy-driven binding processes.	(5)
3.	a)	Distinguish between clatharate and clathrand? What are cucurbiturils? Draw any one cucurbituril.	(5)
	b)	What are calixarenes? Draw the diagram for binding of sodium ion as guest to the oxygen of methyl ether groups of the calixarene and label the hydrophobic part in it.	(5)
4.	a)	Draw the diagrams for Soccer ball" cryptand molecule which acts as a cation host for NH_4^+ ion as well as the diprotonated form acting as a host for H_2O molecule. What makes the soccer ball crypates good hosts for anions?	(5)
	b)	Give any two suitable examples of two-dimensional hosts. Give examples of Zwiterionic hosts and amide based hosts. Which type of hosts can accommodate dicarboxylate anion guests?	(5)
5.	a)	What are the types of interactions that take place when hosts bind with guests? Why are neutral receptors accommodated by hosts?	(5)
	b)	Give the structure of the trimesic acid assembly. Which polyhalogen ions can this network accommodate? What sort of conformation of cyclotriveratrylene helps in forming inclusion compounds in solid state with benzene, toluene etc. Give suitable diagrams.	(5)
6	a)	With the help of a suitable diagram explain the minimal self-replication model which is the key to life.	(5)
	b)	Discuss the mechanism of self-assembly in the Tobacco Mosaic Virus. What are the main non-covalent ineractions that dominate biological self-assembly? Why self-assembly is essential in biology?	(5)
7.	a)	What are the advantageous of having synthetic models of biological systems? Differentiate between a structural mimic and a functional mimic.	(5)
	b)	Describe the three fundamental steps involved in natural and artificial photosynthesis. In what way supramolecular chemistry helps in designing artificial photosynthetic systems?	(5)
8.	a)	Differentiate between catalysis and cocatalysis in supramolecular chemistry. With the help of a suitable diagram give the schematic illustration of the cocatalysis process.	(5)
	b)	What are the essential characteristics of an effective carrier in supramolecular transport? What is electron-cation symport, and how is it achieved in supramolecular transport systems?	(5)
9.	a)	With the help of suitable diagrams give the differences between the structures of racks, ladders and grids.	(5)

b) What are metal-organic frameworks (MOFs)? What are other names of the organic ligands in them. Give examples of any two such frameworks. (5)

10. a) With the help of suitable diagrams explain the synthesis of caternanes and rotaxanes via host-guest chemistry. (5)

b) What is supramolecular isomerism, and how does it relate to polymorphism? Explain the concept of rational design in supramolecular chemistry. (5)

1. a) Explain dipole-dipole interactions in supramolecular chemistry with a suitable example. What is its energy range and why are they important? When are they helpful in molecular recognition? (5)

Answer

Dipole-dipole interactions arise between molecules or groups that possess **permanent electric dipoles**. A polar bond has a partial positive end and a partial negative end. When two such dipoles approach with a favourable orientation, the positive end of one is attracted to the negative end of the other. The interaction falls rapidly with distance, so close contact and correct orientation are important.

For a fixed pair of dipoles, the interaction depends on the product of their dipole moments, their relative orientation and approximately on r^{-3}. After rotational averaging in a fluid it becomes still shorter ranged. For ordinary neutral organic groups, an individual favourable contact is commonly in the **few to a few tens of kJ mol^{-1}** range; about 5-25 kJ mol^{-1} is a useful working range. The exact value changes greatly with distance, geometry and the dielectric constant of the medium.

A simple example is the association of two carbonyl-containing molecules. Each C=O bond has $C^{\delta+}$ and $O^{\delta-}$ ends. An antiparallel arrangement places opposite partial charges close together and is lower in energy than an unfavourable parallel arrangement. Similar effects occur with nitriles, amides and other strongly polar groups.

In molecular recognition these contacts are valuable because they are **directional**. A host can place several polar groups in a preorganised cavity so that only a guest having the correct size, orientation and dipole pattern can make all the contacts at once. They are most useful when the interacting dipoles are well aligned, the host and guest are already shape-complementary, and the binding site is not strongly competed for by a very polar solvent. Several weak dipole-dipole contacts acting together can then give useful selectivity even though one contact alone is modest.