Self-Assembly of Bile Acid Derivatives into Metallosupramolecur Cages

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Natural chiral hydrophobic cavity/pocket containing structures (*e.g.,* metalloenzymes, proteins) are important for many biological functions (*e.g.*, transport, recognition, catalysis). To mimic these natural systems and mechanisms, development of such supramolecular systems (*e.g.*, cages, macrocycles) from chiral natural molecules is required.

Coordination-driven self-assembly is a well-established method to build hollow metallosupramolecular (MSM) structures. However, majority of self-assemblies are made of symmetric, achiral ligands (L) and Pd^{2+}. Recently in our group, first bile acid (BA)-based (ursodeoxycholic acid, UDCA) MSM macrocycles Pd_3L_6 (Figure 1a) were introduced[1] and studied.[2] Beside this, there is only one report about BA-based Pd_2L_4 MSM cages.[3] We further expanded on the family of BAs by synthesizing chenodeoxycholic acid-based ditopic pyridyl ligand, forms a mixture of Pd_nL_{2n} species ranging from Pd_2L_4 to a large Pd_6L_{12}.

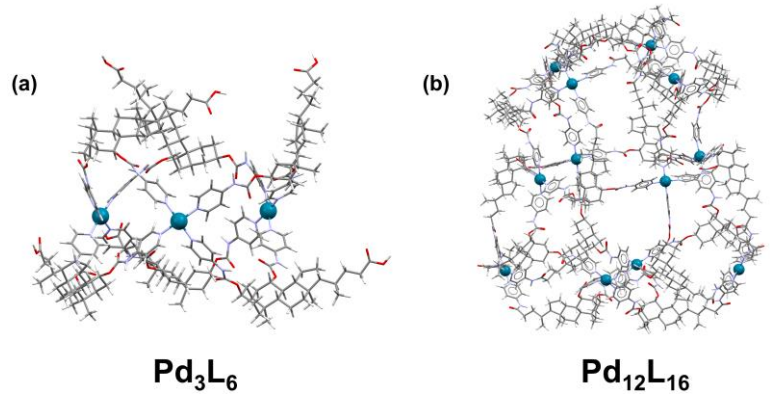

Figure 1. UDCA-based metallosupramolecular a) macrocycle and b) cage.

Thus far, only BA-based ditopic pyridyl ligands were used to prepare MSM systems. Therefore, our latest study presents UDCA-based tritopic pyridyl ligand and its self-assembly with Pd^{2+}, which results in Pd_6L_8 or **first-ever giant $Pd_{12}L_{16}$** (Figure 1b) MSM cage depending on solvent and metal-ligand ratio.

These studies provide better understanding of unsymmetric natural molecule-based ligands self-assembly, effect of their flexibility, topicity, and bend angle in design and construction of chiral cavity containing MSM architectures.

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