Challenges for Supramolecular Crystallography: Metal Organic Nanocapsules

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The enclosure of chemical space is one of the essential attributes of a biological system. However, such enclosures rarely possess long range internal order. As supramolecular assemblies advance toward biological systems in terms of complexity and functionality, the contributions made by supramolecular crystallography become ever more important. As a model for the impact of supramolecular crystallography on the understanding of complex systems, I have chosen metal organic nanocapsules. We have previously shown that macrocycles can serve as building blocks for very large assemblies. In particular, calixarenes and resorcinarenes may be used to enclose space in a manner consistent with the principles of solid geometry attributed to Plato and to Archimedes. The ability of macrocycles to effect the construction of hydrogen-bonded spherical molecular capsules is due to focused functionality. The use of pyrogallol[4]arenes to form hydrogen bonded hexamers and dimers is noteworthy. These hydrogen bonded molecular capsules are both stable and soluble in polar liquids. Recently, we have used Cu^{2+} and Ga^{3+} ions to replace some or all of the hydrogen bonds, affording robust capsules. We have now utilized most of the first row transition metals to seam dimeric and hexameric capsules. In this presentation, the linkage of such metal-seamed capsules in one-, two-, and three-dimensions will be discussed in light of crystallographic challenges.