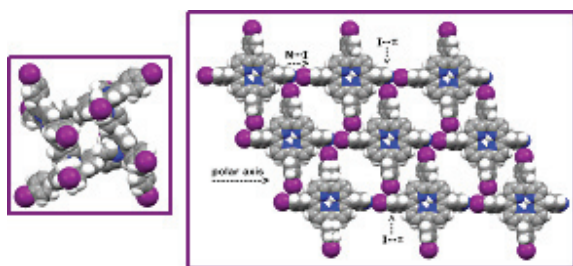


[1].

In the above context, we focus here on porphyrins bearing carboxyphenyl, pyridyl and iodophenyl molecular recognition functions, along with their core-metalated derivatives. This work evaluates the supramolecular reactivity of representative scaffolds, utilizing metal-ligand coordination as well as hydrogen and halogen bond synthons in the construction of polymeric as well as oligomeric structures. It demonstrates also the induction of supramolecular chirality (chiral arrangement of achiral molecular components in a non-covalent assembly), which has been achieved with asymmetrically substituted porphyrin building blocks, using either hydrogen or halogen bonds as directors of the intermolecular organization [2]. Protocols for the rational design of the different modes of supramolecular porphyrin ensembles will be discussed, in relation to the substitution pattern of the recognition sites on the porphyrin moiety.



[1] I. Goldberg, *Chem. Comm.* **2005**, p. 1243; I. Goldberg, *CrystEngComm* **2008**, *10*, 637. [2] S. Muniappan, S. Lipstman, I Goldberg, *Chem. Commun.* **2008**, p. 1777; S. Lipstman, S. Muniappan, I. Goldberg, *Cryst. Growth Des.* **2008**, *8*, 1682.

Keywords: crystal engineering; supramolecular chirality; porphyrin solids

FA4-MS04-O4

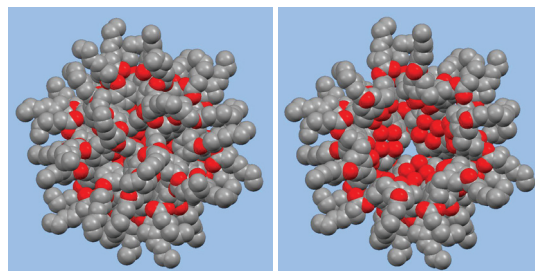
Self-Assembly of Amphiphilic Calixarenes: Crystal Structure of an Inverted Micelle. Kinga Suwinska^a, Barbara Lesniewska^a, Said Jebors^b, Anthony W. Coleman^b. ^a*Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.* ^b*IBCP, CNRS UMR 5086, Lyon, France.*

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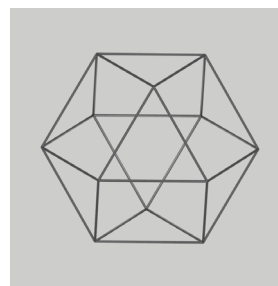
Amphiphilic calixarenes are well known to self-assemble in layers (mono- and bilayers) and/or micelles or inverted micelles. Both, layers and spherical species are of great interest for pharmaceutical and bio-medical applications.

For the first time we were able to observe crystallization of spherical species in the form of inverted micelles and to solve crystal structure of such an assemblies.

12 Calixarene molecules are arranged in cuboctahedron (one of the Archimedean solids) with hydrophobic exterior and hydrophilic internal cavity of 141 Å³.



Inverted micelle: hydrophobic exterior (left) and hydrophilic interior of the inverted micelle. Hydrogen atoms are not shown.



cuboctahedron

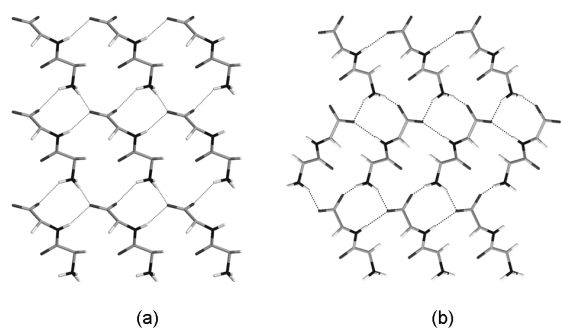
Keywords: amphiphilic calixarene; inverted micelle; structure

FA4-MS04-O5

Head-to-tail Hydrogen-bonded Chains in the Crystal Structures of Dipeptides-A Comprehensive Survey. Carl Henrik Görbitz. *Department of Chemistry, University of Oslo, Norway.*

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At the time when Suresh & Vijayan [1] wrote their classic paper describing head-to-tail sequences as the main mode of interaction between peptide molecules in the solid state, only a limited number of experimental structures were available. The present work provides a comprehensive updated investigation of head-to-tail hydrogen-bonded interactions in the crystal structures of dipeptides, focusing on patterns in which two concomitant chains generate a two-dimensional sheet. It is shown that the presence of such sheets is more abundant than one may initially realize, and furthermore that the vast majority of the observed sheets fall into four well-defined classes, two where molecules in a chain are related only by translation (a), and two where a two-fold screw operation is involved (b). Relating the observed hydrogen bonding patterns to the amino acid composition of the dipeptide, it is clear that the selection between classes is not random; the side chains and even the occasional presence of cocrystallized solvent molecules dictate the outcome of dipeptide crystallization with a high degree of likelihood.



[1] Suresh, C. G., Vijayan, M., *Int. J. Pept. Protein Res.* **1985**, 26, 311.

Keywords: crystal packing; hydrogen bonding; dipeptides