AGGREGATION OF CALIX[4]ARENES USING HYDROGEN BONDING BETWEEN HETEROCYCLES

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One of the fields of supramolecular chemistry which has been gaining attention over the last years is the aggregation of molecules into ordered structures. Hydrogen bonds may play a major role in the controlled association of molecules, not only because of their relatively high strength, but also because of their directionality.

Organization of the hydrogen bond donors and acceptors is the first step towards controlled interaction between molecules. The spacial arrangement of the hydrogen bonds and the amount of hydrogen bonds available for interaction determine for a great part the structure that is obtained. This preorganization of hydrogen bonds is encountered in the nucleotide bases and similar heterocyclic systems. Although interaction between two such units may cause some association, it is expected that multiple hydrogen bonding units are necessary to obtain strong, well-structured aggregates. One of the ways to achieve this is by attaching several units with extensive hydrogen bonding capacity to a platform.

The cyclic calix[4]arene 1 is a versatile molecular platform. It can be easily synthesized in good yield and each of the four phenyl units may be selectively functionalized on the phenolic side (lower-rim) and on the para positions (upper-rim). In our group the two molecules shown below (2, 3) have been synthesized. Both consist of a calix[4]arene with two heterocyclic moieties on the lower rim. Currently the interaction in solution between these two complementary molecules is being studied. Further, the synthesis of calix[4]arenes with different H-bonding units receives attention. (The heterocycles are derivatized to improve their solubility in organic solvents or to cover their functionality until the H-bonding ability is expressed in the final stage.)

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