Pressocucurbit[5]urils: synthesis and supramolecular properties

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Cucurbit[*n*]urils (CB[*n*]) are macrocyclic compounds known for ability to bind organic and inorganic guests in water with high affinity.1 The smallest derivative of this family of compounds - CB[*5*] consist of five glycoluril monomer units and it is able to include only small solvent molecules and gases in its cavity.2 CB[*n*] chemistry was explored almost exclusively in water and acidic media due to limited solubility in organic solvents.

Synthesis and properties of novel macrocycles constructed from propanediurea (Me10prCB[*5*])3,4 and glycoluril (GU1-Me8prCB[*5*])5 unit will be presented. In comparison to other cucurbiturils this compound differs in a shorter carbonyl portals distance and has better solubility in water and organic solvents.

GU1-Me8prCB[*5*] is well soluble in methanol. It allowed us to look deeply into supramolecular chemistry of CB[*n*]s in this organic polar solvent. We described exceptionally strong binding of cations which is even higher than interaction between potassium and crown ethers. The same pressoCB[*5*] derivative exhibits cation-modulated self-assembly into tetrameric aggregate. The tetramer is stabilized by the addition of up to one equivalent of a cation but is fully disassembled in the presence of 2 equivalents of the cation. Cations can thus be used to tune the aggregation of macrocycle in solution.



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