

Poster Presentation

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Phase transformations in cucurbituril host-guest complexes

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The retention of crystallinity upon desolvation of molecular crystals is not common, as the molecules are rigidly and densely packed in the crystals and the original framework usually collapses once solvent is removed from the structure. However, in rare cases the host framework remains substantially unaffected by solvent (guest) removal yielding structure with open channels or discrete lattice voids that can show permanent porosity. [1] Furthermore, sometimes happens, the desolvation process proceeds as single-crystal to single-crystal transformation resulting in distortion and sliding of the structure, changes in conformation, coordination modes and/or space group. Here we would like to present crystallographic study and thermal analysis on the dehydration process of the crystalline supramolecular complex between macrocyclic host cucurbit[6]uril and dopamine. In the solid state the 1:1 host-guest complex assembles into hexameric tubes with water-filled interior channels. Another set of water channels is created between three neighboring tubes in the crystal lattice. The crystals of such supramolecular assembly are not stable when out from mother solution and immediately start to loose water upon exposure to air. However, despite severe cracking the crystals dried in air maintained their integrity and still gave satisfactory diffraction pattern. The X-ray analysis showed significant decrease in the unit cell volume of the partially dehydrated crystals that corresponds to the liberation of some of the water molecules from the channels. Moreover, the reorganization of dopamine guest molecules has occurred in the crystal lattice as a response to the escape of water molecules from the structure. The partial dehydration and reorganization of the supramolecular framework proceeds via a single-crystal to single-crystal mechanism.

[1] L. J. Barbour, *Chem. Commun*, 2006, 1163

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