

LARGE SUPRAMOLECULAR AGGREGATES FROM SMALL CYCLODEXTRINS

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Native cyclodextrins typically cocrystallize with solvent molecules, in addition to the complexed guest species. This phenomenon may lead to a variety of, the so-called, pseudopolymorphism of cyclodextrin complexes. This phenomenon is observed in complexation of chiral guest compounds, namely *cis*-decaline and camphor. Large structures may form containing appreciable amount of solvent, which may be a mixture of chemically different compounds.

In the present paper novel x-ray structures of α -cyclodextrin with camphor and water/methanol (I), β -cyclodextrin with *cis*-decaline and tetrahydrofurane (II), and γ -cyclodextrin with pure water (III) will be presented and discussed. Crystal morphology change which accompanies guest desorption or exchange will be shown as short movies.

All structures have large unit cells, as listed below:

I – $a = 16.17$, $b = 71.97$, $c = 16.45 \text{ \AA}$, $\beta = 119.31^\circ$, $P2_1$, $Z(\text{CD}) = 12$

II – $a = b = 14.847$, $c = 72.41$, $P4_122$, $Z(\text{CD}) = 16$

III – $a = 20.236$, $b = 32.774$, $c = 33.814 \text{ \AA}$, $\beta = 105.22^\circ$, $P2_1$, $Z(\text{CD}) = 12$

Disorder of guest species and solvent molecules adds to complexity of the crystal structures and, what produces particular problems in crystal preparation for x-ray data collection, the crystals show pronounced abilities to exchange its complexed guest/solvent species when exposed to variable environment.

The structure of solvation patterns will be discussed and related to the zeolitic behaviour of the solids.

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