Different Building Modes of α-Cyclodextrin/Monoalkyl Amphiphile Complexes

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In this study, the impact of the length of the guest molecule alkyl chain and the crystallization conditions on the structural parameters of α-cyclodextrin (α-CD)/monoalkyl complexes was determined. Several procedures to crystallize those complexes were developed for different alkylalcohols as model guest molecules, as a function of temperature. Three different crystalline structures were identified depending on the alkyl chain length, using synchrotron X-ray diffraction (LURE, Orsay, France). In all cases, complexes crystallize in channel-type structures, where α-CD molecules are stacked like coins in a roll and the alkyl chain of the guest compound is embedded in the tubular cavity of the α-CDs. However, depending on the length of the chains and the crystallization conditions, the channels are organized differently. C_6-C_8 chains give rise to a pseudo-hexagonal lattice, a packing mode already observed for polyiodide complexes [1]. C_{10}-C_{12} chains crystallize in a triclinic pseudo-monoclinic C2 lattice, while longer chains up to C_{18} form hexagonal crystals with R3 symmetry. These two novel crystal structures are described. Understanding these structures opens new routes to nanotube formation through amphiphile-driven crystallization of cyclodextrin templates.

[1] Noltemeyer M., Saenger W., *J. Am. Chem. Soc.*, 1980, **102,** 8, 2710.

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