

Unusually high efficiency of β -cyclodextrin clathrate preparation by water-free solid-phase guest exchange

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Abstract

An effective preparation procedure is offered for β -cyclodextrin (bCD) clathrates with volatile guests of moderate hydrophilicity, which otherwise require a finely tuned optimization of the bCD/water/guest ratio. The proposed procedure includes guest exchange in a water-free bCD matrix. As a result, more stable clathrates with a higher inclusion capacity can be prepared than by direct saturation of dried or hydrated bCD. To find an optimal preparation method, the structure-property relationships were studied for four different ways of bCD clathrate formation with guests of varying molecular structure. The study was much simplified by used procedures excluding direct contact of guest and water liquids with bCD. Besides, in clathrate preparation experiments, the thermodynamic activities of water and guest were varied independently, which makes explicit the role of water in this process. Hydration of bCD reduces its inclusion threshold for hydrophobic guests by their activity (relative vapor pressure), giving favorable hydration effect for their inclusion. Besides, water competes with hydrophilic guests for binding sites in bCD at high water activities. Together with bCD dehydration by excess of hydrophilic guests, these observations give a complete thermodynamic picture, which may be fruitful for elaboration of guest encapsulation techniques by cyclodextrins. © 2013 American Chemical Society.

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