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Structure and stability of oligomer/α-cyclodextrin inclusion complexes. MARCUS HUNT, North Carolina State University, SILVIA VILLAR, MARIAN GOMEZ, Institute of Polymer Science and Technology, CSIC, Spain, ALAN TONELLI, MAURY BALIK, North Carolina State University — Cyclomaltohexaose (α-cyclodextrin, α-CD) can form inclusion complexes (ICs) with polymer molecules in the columnar crystal in which α-CD molecules stack to form a molecular tube. Complementary water vapor sorption and wide-angle X-ray diffractomery (WAXD) were performed on oligomer/α-CD ICs to probe their structures and stabilities. To discern the effect of guest molecule hydrophobicity on water adsorption isotherms, polyethylene glycol (PEG, MW = 600 g/mol) and hexatriacontane (HTC) guests were used. Sorption isotherms for PEG/α-CD IC are similar to those obtained for pure α-CD and PEG, suggesting the presence of dethreaded PEG in the sample. WAXD collected before and after water vapor sorption of PEG/α-CD IC indicated a partial conversion from columnar to cage crystal structure, the thermodynamically preferred structure for pure α-CD, due to dethreading of PEG. This behavior does not occur for HTC/α-CD IC. Sorption isotherms collected at 20, 30, 40 and 50 $^\circ$ C allowed the calculation of differential heats of adsorption and integral entropies of adsorbed water, while solid-state ^{13}C NMR suggested a dramatic increase in HTC and α-CD mobilities upon complexation.

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