



Discrete cuboidal 15- and 16-membered water clusters in brucine 3.86-hydrate, water release and its consequences.

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Streszczenie

Up to now, three brucine hydrates are known, brucine di-, tetra-, and 5.25-hydrate. All of them were obtained from solutions containing the additive diethanolamine, adenosine, and urea, respectively. Studying the role of the additives on crystallization of the brucine hydrates, we obtained a new, kinetically favored brucine 3.86-hydrate. In crystals of brucine 3.86-hydrate, large 15- and 16-membered water clusters of cuboidal topology are encapsulated in cages formed between honeycomb-like brucine layers. Dehydration of the brucine hydrate leads to formation of the known anhydrous brucine, giving insight into a mechanism of the dehydration process, in which a shift of brucine ribbons in the honeycomb-like layers leads to an opening of channels and water release. A collapse of brucine layers after the water release results in formation of the common anhydrous brucine. The anhydrous brucine undergoes a phase transition at 249 K in the cooling mode and at 277 K in the heating mode. The phase transition is attributable to a huge shift of brucine corrugated layers in relation to each other. The phase transition for anhydrous brucine obtained by dehydration is accompanied by thermal effects one order larger than anhydrous brucine, obtained by crystallization from acetone solution.

Adres publiczny

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Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>