MS34 Molecular recognition, supramolecular chemistry and crystal engineering

Chairs: Chiara Massera, Carl Henrik Görbitz

MS34-P1 Crystallization *in situ*, structural investigation, physicochemical properties of azetidine cocrystals with water

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The purpose of this study was to device, obtain and determine the structures of cocrystals of azetidine with water. Azetidine is volatile liquid cyclic secondary amine with four membered ring. The crystal structure of the neat amine is known [1]. There is also an evidence that azetidine can co-crystallize with water and form sI type clathrate hydrate [2]. Using IR laser assisted *in situ* crystallization technique [3] two unknown polymorphs of azetidine and four hydrates were obtained. Azetidine forms hemi- and monohydrate crystal phases as well as two hydrates containing seven and twelve water molecules per one amine molecule. Hemihydrate has two transformation polymorphs with phase transition at the temperature below 170 K. In hepta- and dodecahydrates amine molecules interact with water lattice *via* non-covalent, hydrogen bonds N-H…O. Comparing unit cell parameters, crystal structure of heptahydrate can be considered as sI clathrate [4]. Information obtained from the X-ray diffraction experiment shown however that water molecules form three distinct cages what results is a new type of hydrate. Moreover heptahydrate crystallizes in different, Pm-3 space group than clathrate hydrate type sI which is Pm-3n. The comparison of azetidine hepathydrate crystal structure and clathrate hydrate type sI is presented in the figure below. Additionally all obtained solid phases were characterized with use of the Raman spectroscopy.

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References

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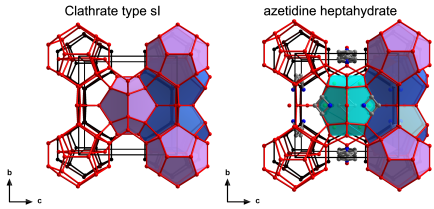

Figure 1. Crystal packing comparison of hydrate clathrate type sI and azetidine heptahydrate

Keywords: Hydrates, Clathrahes, Azetidine, in situ crystallization, Crystal Engineering, Single Crystal Diffraction, Raman Spectroscopy