

## MS34-P11 Structural and spectroscopic investigations of cyclobutylamine and cyclobutylamine hydrates

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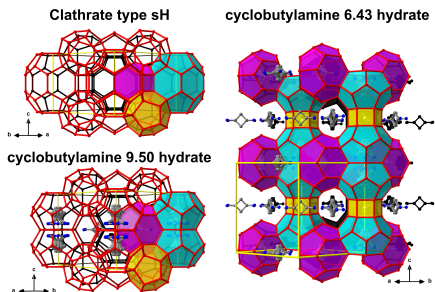
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Clathrate hydrates are fascinating group of compounds where the guest molecules are trapped in the water cage. The most known example are clathrate hydrates of methane [1]. This research is focused on the supramolecular synthesis of compounds of this kind with cyclobutylamine as the guest molecule. The structure of the amine hemihydrate is already known. It crystallizes in monoclinic  $P2_1/n$  space group [2]. The crystal is stabilized by a hydrogen bond and weak van der Waals interactions. To screen the possibility of hydrate/clathrate formation and the amine/water ratios some preliminary XRD experiments have been made. The samples suitable for single crystal X-ray diffraction were grown with use of the *in situ* crystallization method assisted by IR laser [3]. In this way we were able to obtain crystals of the cyclobutylamine and its four new hydrates containing: 1.00, 6.43, 7.54 and 9.50 water molecules *per* one amine molecule [4]. Their crystal and molecular structures were solved with use of the X-ray diffraction experiment on single crystal. The structures containing larger amount of water (6.43, 7.54 and 9.50 hydrates) resembled clathrate hydrates of methane. Contrary to true clathrates the guest molecules interacted with the water framework via N...O hydrogen bonds. These structures are in addition severely disordered. All systems were also characterized using Raman spectroscopy.

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### References

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**Figure 1.** Packing diagrams of 6.43 and 9.50 hydrates of cyclobutylamine compared to structure of clathrate type sH

**Keywords:** Hydrates, Clathrates, Cyclobutylamine, *in situ* crystallization, Crystal Engineering, Single Crystal Diffraction, Raman Spectroscopy