

# Poster Presentations

## [MS24-P36] Structural investigations on water and *tert*-butylamine system

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Gas hydrate clathrates is very interesting and important group of compounds. In the structure of such systems water molecules form voids able to host some guest moieties like methane. In these types of crystals only weak dispersive interactions occur between water framework and guest molecules. It is believed that more methane is trapped in hydrate clathrates located on the beds of seas than can be found in traditional deposits. Such crystals occurring in nature are stable under certain pressure and temperature conditions only. So gas clathrates could serve as a huge source of methane but the excavation process must be very careful – methane is strong greenhouse effect agent. Gas clathrates can also cause serious problems while blocking pipelines [1]. Therefore there is huge interest in research on gas clathrates to make such systems more stable or to prevent their formation. [2].

But not only hydrocarbons can form gas clathrates. There are known examples of other molecules like THF [3] or some amines [4] forming clathrates. Is it really so that primary or secondary amines, being a potential hydrogen bond donor and/or acceptor, are not a good partner for water molecules to interact? From the CSD [5] one can find interesting example of amine clathrate – cubic structure of *tert*-butylamine [6], however with a relatively high discrepancy factor. The other known hydrate of this amine has strong HB interactions [7]. To

reveal the secrets of this system and check if *tert*-butylamine interacts with H<sub>2</sub>O molecules we decided to co-crystallize *tert*-butylamine with water. Because both ingredients are liquids at ambient conditions we grew all the crystals on the goniometer head of the diffractometer using *in situ* laser crystallization technique [8]. As the result of our experiments we obtained pure amine and 7 crystalline hydrates, 5 of them new. We found that in all obtained structures amine interacts with water molecules thus none of such system should be regarded as clathrate. Our single crystal structural investigations were supported by *in situ* Raman spectroscopy experiments.

### References:

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