

MS34-P16 Structural chemistry of piperidine hydrates

Paweł Socha¹, Lukasz Dobrzycki¹, Michał K. Cyrański¹, Roland Boese¹

1. Czocharlski Laboratory of Advanced Crystal Engineering, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-093 Warsaw, Poland

email: psocha@chem.uw.edu.pl

The aim of this report was to investigate the possibility of creating hydrates or clathrates for piperidine-water system. Piperidine is a heterocyclic aliphatic amine with six-membered ring. Crystal structure of the amine is known, molecules build columns in crystal lattice [1]. Hydrates were crystallized on the diffractometer, using *in situ* crystallisation technique with IR laser [2]. Five hydrates have been received during the project, consisting of 0.50, 2.00, 8.10, 9.75 and 11.00 water per one amine molecule. Structures of hydrates were determined with single crystal X-ray diffraction. Interestingly, hydrates with high concentration of water were very similar to gas clathrates [3], however there were hydrogen bonds between amine and water in crystal lattice and the water framework including positions of H₂O molecules was disordered. What is more, piperidine hydrates consisting 9.75 and 11.00 water were isostructural with an analogue structure of *tert*-butylamine hydrates [4, 5]. Packing diagrams of these two structures are presented in the Figure below. Moreover, piperidine hydrate 8.10 were isostructural with *iso*-propylamine hydrate 8.00 [6, 7]. All synthesised crystals were also characterised with Raman spectroscopy and X-ray powder diffraction.

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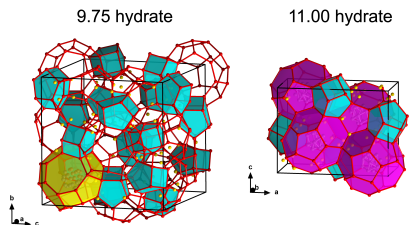


Figure 1. Unit cell content of 9.75 and 11.00 hydrates of piperidine. Alternative positions of H₂O molecules indicating disorder of water framework are presented as yellow spheres.

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