MS32-P116 - LATE | MOLECULAR INTERACTION IN HYDRATES OF 4-METHYLPIPERIDINE AND 4-CHLOROPIPERIDINE

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Piperidine is an aliphatic, heterocyclic amine consisting of a six-membered ring. The crystal structure of the amine is known [1]. Our previous research shown that piperidine tends to form several crystalline hydrates with different amounts of water [2]. Importantly, the hydrates with high concentration of water have very similar structures to gas clathrates [3].

The aim of this research was to investigate the impact of the substituent in the piperidine ring on the hydrate formation and to analyze the architecture of obtained structures. Hydrates were grown at ambient pressure, directly on the single crystal diffractometer using IR laser supported *in situ* method [4]. As a result the following phases were obtained: hemihydrate and trihydrate for 4-methylpiperidine and monohydrate and trihydrate for 4-chloropiperidine. Interestingly, both trihydrates have the same L4(6)5(7)6(8) [5] water-layer motif and both melt around 263 K. However, amine-water hydrogen bonds in these crystals are different. Moreover, in the 4--chloropiperidine hydrate halogen-halogen interactions can be found. Among analyzed piperidine derivatives no high water content systems similar to clathrate hydrates were observed what can be attributed to inappropriate shape and size of the investigated molecules.

[1] A.Parkin, I.D.H. Oswald, S.Parsons, *Acta Crystallogr.,* **2004**, *B60,* 219-227.
[2] Ł.Dobrzycki, P.Socha, A.Ciesielski, R.Boese, M.K.Cyrański, *Cryst. Growth Des.,* **2019**, *19,* 1005−1020.
[3] E.D. Sloan, "*Clathrate Hydrates of Natural Gases",* Marcel Dekker, New York, USA, **1990**.
[4] R.Boese, *Z. Kristallogr.*, **2014**, *229*, 595−601.
[5] L.Infantes, S.Motherwell, *CrystEngComm*, **2002**, *4,* 454−461.