MS30 Hydrogen bonding from theory to applications

Chairs: László Fábián, Nikoletta Bathori

MS30-P1 Towards an Understanding of Hydrate Formation

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Hydrates constitute an important class of multicomponent crystals pertinent to both crystal engineering[1-3] as well as pharmaceutical science[4]. The occurrence of hydrates in molecules containing solely strong H-bond donors or H-bond acceptors in particular has thus far been understudied. A comprehensive investigation of hydrate formation in *N*-heterocyclic aromatic compounds that lack strong H-bond donor groups was therefore performed. A Cambridge Structural Database (CSD) survey of 5- and 6-membered *N*-heterocyclic aromatics, and hydrate screening experiments on a small set of compounds **1-11** (Figure 1) were conducted. The hydrate screening experiments involved: (i) crystallization from mixed solvent systems, (ii) slurry in water at ambient temperature, and (iii) exposure of anhydrous form to humid conditions (75% relative humidity at 40 °C). The results, which, when coupled with modelling experiments, provide much needed insights into the formation of hydrates and will be detailed.

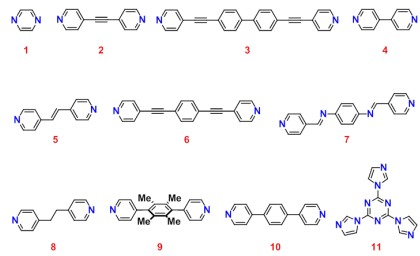

Figure 1. *N*-heterocyclic compounds investigated for hydrate screening.

Keywords: Crystal engineering, hydrogen bonding, hydrate screening

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