

MS34-O3 Solvent dependence of competitive hydrogen vs halogen bonded self-assembly processes in multi-component crystal formation

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A series of experiments were carried out which directly contrasted the ability of hydrogen and halogen bonding (HB & XB, respectively) to drive a self-assembly process and the effect that solvent has on this process. This was achieved in a competitive environment in which either a two-component HB network or a two-component XB network may co-crystallise from a system of three small organic molecules (HB donor, XB donor and acceptor). The experiments were carried out in seven solvents of different polarities, ranging from toluene to *i*-propanol. The identity and phase purity of the products was analysed by single crystal and powder X-ray diffraction. The investigation revealed that the network formed by co-crystallisation is indeed solvent dependent, with HB networks formed in lower polarity solvents, switching to XB networks in solvents of higher polarity. By adjusting the strength of the HB donor relative to the XB donor we were able to gain further solvent-dependent control and ultimately reverse the network selectivity in all solvents. These results reveal the solvent-dependent nature of Metrangolo and Resnati's original HB vs XB co-crystallisation experiment and demonstrate that the nature of the solvent is an important consideration and may offer a further level of control of the fidelity of self-assembly processes.

1. E. Corradi, S. V. Meille, M. T. Messini, P. Metrangolo and G. Resnati, *Angew. Chem. Int. Ed.*, **2000**, *39*, 1782-1786

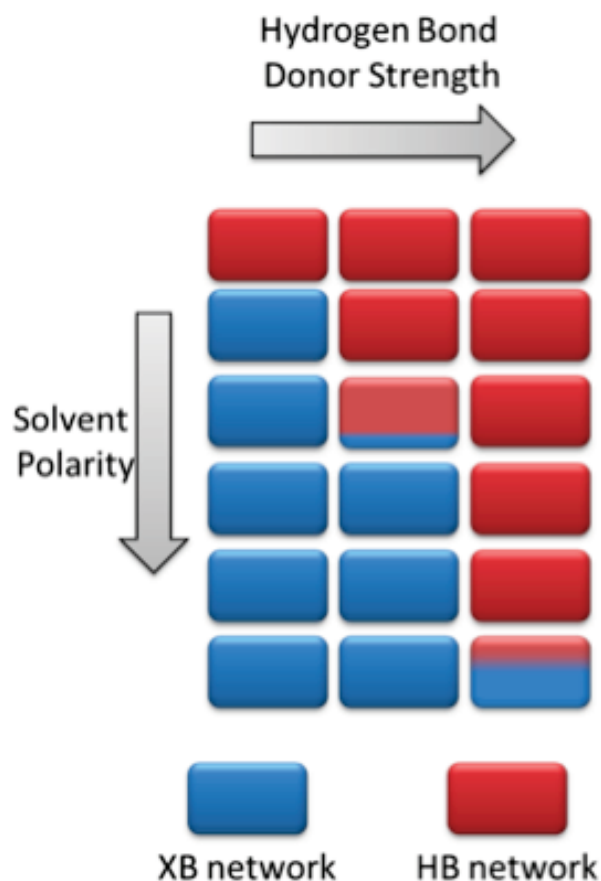


Figure 1. The outcome of a competitive co-crystallisation between a HB vs XB network in seven solvents is affected by both the nature of the solvent and the HB strength of the donor.

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