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Searching the Cambridge Structural Database for solvated vs. unsolvated pairs

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E-mail: streek@ccdc.cam.ac.uk**Keywords:** solvates, hydrates, cambridge structural database

The more than 365,000 organic and organometallic small-molecule crystal structures in the Cambridge Structural Database (CSD) are a good source of data for understanding the crystal structures of solvates. It is trivial with the existing search software [1] to find all CSD entries containing a particular solvent, say water, and a survey of the 50 most common solvents in the CSD has been published [2]. It might be interesting, however, to know if any of these solvates also exist in an unsolvated form; given a crystal structure of di-isopropylammonium chloride hydrate in the CSD, for example, one could wonder if a crystal structure of di-isopropylammonium chloride itself is present in the database.

A computer program was written that for a given solvent molecule finds all pairs of solvated *versus* unsolvated CSD entries; a list of solvate structures for which no unsolvated form exists in the CSD is also generated. These lists enable us to examine if properties such as the number of hydrogen-bond donors / acceptors or the molecular flexibility influence solvate formation. Results for hydrates will be presented.

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Constructing co-crystals with molecular sense and supramolecular sensibility

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What is most likely going to happen when a homogeneous solution containing two different molecular solutes is allowed to evaporate to dryness? Unless a chemical reaction driven by the formation of covalent bonds takes place between the two solutes one would, as a rule, expect the appearance of two separate molecular solids. This is a manifestation of the inherent structural selfishness of molecules, something that is relied upon every time recrystallization is employed as a method of purification. Recrystallization processes are essential in most covalent synthetic procedures and are performed on a regular basis in every synthetic laboratory. In the supramolecular laboratory, however, the very same process also provides an opportunity to move in the opposite direction - a co-crystallization is a deliberate attempt at bringing together different molecular species in one crystalline lattice without making or breaking covalent bonds. Recrystallization and co-crystallization processes are, in essence, only distinguishable by their intents. Since the odds are stacked firmly in favor of a homomeric product, how do we go about developing reliable and versatile synthetic methods for the directed assembly of co-crystals? This presentation will attempt to answer the question by outlining several modular hydrogen-bond driven strategies for the design and synthesis of binary and ternary supermolecules and co-crystals [1-3].

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