Poster

Structural studies of urea clathrates with aliphatic diamines

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Urea is an incredibly intriguing molecule due to its extensive applications in various fields, including pharmacy, agriculture, and industry. From structural point of view it exhibits a significant versatility in forming a wide range of systems, from simple ones to highly complex compounds, including macrocycles. Arguably most interestingly, it has the ability to form channel clathrates with linear molecules such as aliphatic hydrocarbons and their derivatives.

The first documented example of such clathrate is the urea-1-octanol system. The exploration of its structures began in the 1980s. These clathrates exhibit an architecture of hexagonal infinite channels, where guest molecules are loosely bound. Moreover, they are often highly disordered. Crystallization of these compounds typically take place in the $P6_1$ or $P6_5$ space groups, resulting in enantiomorphic crystal forms. This phenomenon arises from the formation of helical structures, facilitated by the hydrogen bonds formed between urea molecules and their neighboring counterparts.

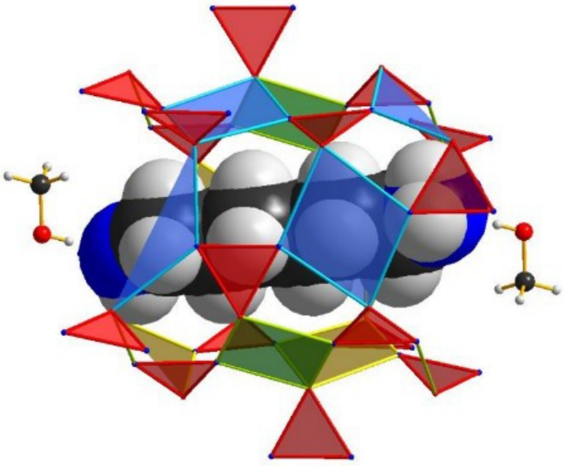

Figure 1. Urea clathrate with 1,6-diaminohexane

The aim of this presentation was a synthesis and structural characterization few six urea finite urea clathrates with 1,*n*-diaminoalkanes (where $n = 3 \div 8$). These clathrates form channels whose length is related to the dimensions of the diamines. The amine groups interact, by hydrogen bond, with a solvent molecule, methanol, leading to stabilization of the system. Interestingly, in addition to chiral tubes composed of urea molecules, centrosymmetric ones can also be formed. The variation in topology observed in these systems can be attributed to the presence of a minimal motif consisting of four urea molecules. This motif gives rise to a distinctive rhombus shape, with the edges formed by hydrogen bonds between the four urea molecules. The relative arrangement of these molecules determines whether the resulting system is chiral or centrosymmetric. Importantly, it has been demonstrated that the topology of urea channels in these clathrates is governed by this fundamental motif, ultimately influencing the overall crystal architecture.

[1] M. F. Bengen, *Angew. Chem*., **6** (1951) 207.