MS29-2-1 Co-crystals of n-alcohols with propyl-, allyl- and propargylamine. Effect of C-C bond saturation on the structural motifs
#MS29-2-1

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Abstract
Amines and alcohols can act as good ingredients for the co-crystallization experiments. This is due to the complementarity of their functional groups in terms of hydrogen bonds formation. In the literature there are known some examples of such structures but they are mostly limited to diamine-diol co-crystals [1] or aromatic systems [2]. The presented here results are focused on the influence of C-C bond saturation in the small amine molecules on the co-crystals formation with n-alcohols. As the simplest and stable unsaturated compounds allylamine and propargylamine were chosen. The reference molecule was propylamine. In such model systems, both intra- and intermolecular interactions are not affected by the presence of additional substituents and functional groups.
The examined mixtures are liquid under ambient conditions, therefore an IR laser-assisted in situ crystallization technique was used to obtain desired co-crystals directly on the goniometer of the single crystal diffractometer [3]. The X-Ray measurements were complemented by DFT periodic calculation in CRYSTAL17 program.
During the research 30 mixtures were tested (ten alcohols in methanol-decanol range with three amines) for which 25 co-crystals were obtained. In the structures three types of hydrogen bonds motifs are observed. Two different layers of L4(4)8(8) and L6(6) types and ribbon T4(2) [4]. Elongation of the aliphatic chain of the alcohol causes the change of the motif in a systematic way. However the point of transition is different for various amine, due to the influence of the C-C bond saturation.
To elucidate the influence of the saturation of the C-C bond on the formation of co-crystals, several periodical calculations were performed. They were based on the cohesive energy calculation combined with its partition to the interactions within structural motifs and among them. This type of computation allows to compare structures with 1D and 2D motifs and help to understand the reasons why a particular architecture is observed. A finite number of potential motifs made it possible to model the structures of unobtained co-crystals, to verify their energy properties.
Systematic research of amine-alcohol co-crystals shows that changes in structural motifs are predictable in the studied group. The known properties can be used to design similar systems.

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