Hydrogen bond architecture in a series of allylamine and normal alcohols (C_1-C_{10}) cocrystals

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Alcohols and amines can be considered as excellent cocrystal forming agents, due to the compatibility of intermolecular interactions where both compounds act as hydrogen bond donor and acceptor. In such structures different motifs as isolated oligomers (0D), ribbons (1D), layers (2D), etc. can be expected. The main trust of the research was the crystallization and structure determination of cocrystals of allylamine and alcohols followed by the analyses of hydrogen bond architectures, using computational methods.

The examined mixtures are liquid at ambient conditions, therefore, an IR laser-assisted *in situ* crystallization method has been used directly on the goniometer of the single crystal diffractometer [1]. The X-Ray measurements were complement by DFT periodic calculation in CRYSTAL17.

Among obtained cocrystals, those with three simplest alcohols (methanol, ethanol, and 1-propanol) contain molecules arranged in layers with L4(4)8(8) motif [2] of hydrogen bonds. Further elongation of the aliphatic chain of the alcohol moiety leads to change in hydrogen bonds architecture from 2D to 1D. In consequence, all cocrystals containing C_4 to C_7 alcohols infinite ribbons reveal the T4(2) topology [2]. Further modification appears for 1-octanol cocrystal, where the molecules interact *via* hydrogen bonds forming layers of the L6(6) type [2]. Thus different topology than for C_1-C_3 alcohols is observed. This structural motif is preserved for cocrystals with C_9 and C_{10} alcohols.

In the analyzed structures three types of hydrogen bonds motifs occur, depending on the aliphatic chain length of the alcohol molecule. Furthermore, all the systems were analyzed according the binding energy between structural units (ribbons or layers) present in the structures. In addition the calculations were also performed for simulated structural units (e.g. applying 1D motif for methanol and 2D motif in case of butanol) to show a potential reason for specific architecture type formation in analyzed cocrystals.

The research shows that for ten allylamine – alcohol cocrystals three of structural motifs may exist. Elongation of the aliphatic chain of the alcohol impacts on the change of the motif in a systematic way. This alteration can be used for rational design of similar systems.

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