MS29-2-9 Synthesis and structural studies of cocrystals of cis and trans isomers of 1,2-cyclohexanediol with selected amines
#MS29-2-9

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Abstract
Presented work is dedicated to crystal engineering [1] of aliphatic and aromatic amines and isomers of 1,2-cyclohexanodiol. When crystallization experiments with small molecule aliphatic amines or aniline are performed at ambient conditions the formation of neat crystalline diol is observed. The only exception is formation of co-crystal with *trans*-1,2-cyclohexanediol and 4-fluoroaniline at room temperature. Hence, to analyze crystallization behaviour of the title diol with series of amines (cyclopropylamine, cyclobutylamine, cyclopentylamine, cyclohexylamine, propylamine, butylamine, isobutylamine, *tert*-butylamine, aniline, ethylenediamine) *in situ* method supported by IR laser was used [2]. The crystals grown directly on the goniometer head were characterized by single crystal X-ray diffraction technique. It is observed that the *trans* isomer of 1,2-cyclohexanediol forms cocrystals with amines more willingly than the *cis* variant. In some cases plastic phases are formed. In all the obtained cocrystals hydrogen bonds between amino and hydroxyl groups are the main intermolecular forces that determine the crystal structure. In the co-crystal of *cis*-1,2-cyclohexanediol with cyclobutylamine the molecules are arranged in columns. In the remaining twelve systems, the structural motifs can be classified as layers, among which it is possible to distinguish different topologies of N…O interactions. The similarity of the structural motifs in the resulting crystal phases suggests that some predictability can be expected in the organization of molecules in systems composed of similar diols and amines. This fact makes these compounds very useful building blocks for crystal engineering and supramolecular recognition [3].

References
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