MS27-P110 - LATE | TOWARDS PHASE TRANSITION IN COCRYSTALS OF ALLYLAMINE WITH

ALIPHATIC ALCOHOLS

Nowosielska, Bernadeta (University of Warsaw, Faculty of Chemistry, Czochralski Advanced Crystal Engineering Laboratory, Warsaw, POL); Cyranski, Michal (University of Warsaw, Faculty of Chemistry, Czochralski Advanced Crystal Engineering Laboratory, Warsaw, POL); Boese, Roland (University of Warsaw, Faculty of Chemistry, Czochralski Advanced Crystal Engineering Laboratory, Warsaw, POL); Dobrzycki, Lukasz (University of Warsaw, Faculty of Chemistry, Czochralski Advanced Crystal Engineering Laboratory, Warsaw, POL)

Alcohols and amines can be considered as excellent cocrystal forming agents. This is due to compatibility of the intermolecular interactions where both compounds can act as hydrogen bond donor and/or acceptor. In such structures different energy-efficient structural motifs as isolated oligomers (0D), ribbons (1D), layers (2D) etc. can be expected. The aim of the research was to investigate cocrystallization of allylamine with selected aliphatic alcohols (methanol, ethanol, 1-propanol, 2-propanol, cyclobutanol, 1-butanol, *tert*-butanol), analyze structural motifs and check dynamic of the molecules in the obtained systems. The examined mixtures are liquid at ambient conditions, therefore, a laser-assisted *in situ* crystallization method directly on the goniometer of the single crystal diffractometer was used [1].

Among obtained cocrystals those with methanol, ethanol and 1-propanol contain molecules arranged in layers with L4(4)8(8) motif [2] of hydrogen bonds. In systems with other alcohols formation of 1D ribbons of hydrogen-bonded molecules are observed. Change of the crystal architecture can be attributed to the larger size of aliphatic group of the alcohols acting as a steric hindrance what is clearly visible in disordered structure with *tert*-butanol. Here a discrepancy between the size of cocrystal components lead to reversible order-disorder phase transition at lower temperatures with fragmentation of hydrogen bond chains, turning crystal architecture to 0D.

The research was supported by the National Science Center in Poland (Grant SONATA BIS 6 NCN, 2016/22/E/ST4/00461).

- [1] R. Boese, Z. Kristallogr., 2014, 229, 595-601.
- [2] L. Infantes, S. Motherwell, CrystEngComm, 2002, 4, 454-461.