

MS36-P132 - LATE | POLYMORPHISM IN IONIC CO-CRYSTALS - STRUCTURAL CHARACTERIZATION

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Ionic co-crystals (ICC) are usually formed by organic molecule and inorganic salt. This class of compounds can combine properties of its components; e.g. bioactivity of organic molecule and good solubility of the salt, because of which it become of interest for crystal engineering and pharmaceutical applications. It was observed, that LiX-aminoacid ICCs can form structures of square grid topologies, build of 16-membered rings [1,2]. Whole networks are labile, and thus prone to polymorphs formation. Herein we present $\text{LiClO}_4 \cdot 2\beta\text{Ala}$ systems with both chiral and centrosymmetric basic motives, emerging from achiral components, crystallizing in $P2_1$ and $Pbca$ space groups, respectively. What is more, ICCs were found to exhibit polymorphism with chiral – achiral solution – assisted phase transition analysed with PXRD and DSC experiments. Both polymorphic forms were structurally characterized using single-crystal X-ray diffraction showing topological similarity. Thermal tensor of kinetically and thermodynamically preferable forms was investigated, showing difference in thermal behaviour of both polymorphs. Periodic calculations allowed for confirmation of lattices energy differences in both structures.

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[1] Baran, J., et al., J. Mol. Struct. 927, 1-3 (2009) 43-53.

[2] Ong, T. T., et al., J. Am. Chem. Soc. 133, 24 (2011) 9224-9227.