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Structural aspects of partial solid solution formation: Two crystalline modifications of a chiral derivative of 1,5-dihydro-2: H -pyrrol-2-one under consideration

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Abstract

The purposeful change of crystallization conditions for rac-3-chloro-5-hydrox--1-(4-methylbenzyl)-4-[(4-methylphenyl)sulfanyl]-1,5-dihydro-2H-pyrrol-2-one 1 leads to two different crystal modifications, namely, a racemic compound in the triclinic space group P1 with Z′ = 1 (α-1) and a partial solid solution based on a racemic compound in the monoclinic space group P2 1 with Z′ = 4 (β-1). The first modification, α-1, is characterized by a higher density of the molecular packing in the crystal, while the second one, β-1, by a stronger system of hydrogen bonds and the presence of positional and substitutional disorder simultaneously. The analysis of the crystal structure of modifications α and β allowed us to define some structural aspects of the partial solid solution formation. Namely, the tendency to build a stronger hydrogen bond system enables the solution of enantiomers of 1 to be formed in the crystalline phase, whereas the propensity of the molecules to adopt a more favorable transoid conformation limits the solubility of the minor enantiomer. 2017 The Royal Society of Chemistry.

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