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S=O...S=O Interactions as a Driving Force for Low-Temperature Conformational Rearrangement of Stable H-Bonding {S(O)-CH₂-CH₂-OH...}₂ Synthon in two Modifications of Diastereomeric Pinanyl Sulfoxides Co-Crystal

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Abstract

Copyright © Taylor & Francis Group, LLC. (Graphical Abstract) For the triclinic and monoclinic modifications of diastereomeric pinanyl sulfoxides co-crystal, remarkable alterations in unit cell parameters by transition from 293 to 150 were ascertained. Such alterations are accompanied by conformational restructuring of a stable hydrogen-bonded synthon from an "unfolded" to a "folded" form. The driving force of this restructuring is the tendency to form S=O...S=O interactions, which show up in the lower temperature phases of both polymorphs. These are well-supported by the methods of quantum chemistry (DFT, B97-D/6-31G(d,p), AIM All).

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Keywords

"racemic compound-like" crystallization, -β-pinene, hydrogen-bonded cyclic dimers, lower temperature X-ray structural analysis, polymorphic modifications, β-Hydroxy sulfoxide