

Phosphorus, Sulfur and Silicon and the Related Elements 2014 vol.189 N5, pages 615-629

Study of "racemic compound-like" behavior of diastereomeric mixture of pinanyl sulfoxides by x-ray diffraction, ir spectroscopy, and DFT calculations

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Abstract

The oxidation of a β -hydroxysulfide in the pinane series by use of mchloroperbenzoic acid resulted in the formation of the corresponding β -hydroxysulfoxide as a mixture of two diastereomers in 4:5 ratio. According to single-crystal X-ray diffraction (XRD) results, it is established that the diastereomeric mixture of sulfoxides crystallizes in the "racemic compound-like" manner under formation of asymmetric dimers through S=O \cdots H-O interactions. This asymmetric dimer formed from diastereomeric molecules is a structural unit in both crystal modifications, the triclinic and the monoclinic one. The behavior of the diastereomeric mixture of pinane derived sulfoxides in crystals, melts and in tetrachloromethane solutions was studied by IR spectroscopy. The density functional theory (DFT) method with 6-31G (d, p) basis set was used to calculate the optimized geometrical parameters and vibrational frequencies of different associates in solution. The calculated vibrational frequencies are compared with experimental IR spectra. Copyright © 2014 Taylor & Francis Group, LLC.

<http://dx.doi.org/10.1080/10426507.2013.843003>

Keywords

"Racemic compound-like" crystallization; XRD structure determination, (-)- β -pinene, Hydrogen-bonded cyclic dimers, Polymorphic modifications, β -Hydroxysulfoxide