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Crystallization of racemic 4-arylsulfonyl-2(5H)-furanones: Reproducibility of homochiral associates, conditions for the spontaneous resolution of enantiomers and the formation of racemic compounds, the role of intermolecular interactions

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Abstract

Crystallization of three 4-arylsulfonyl-2(5H)-furanones from chloroform leads to the formation of a conglomerate of sulfone with para-tolyl substituent and racemic crystals of chloro and bromo analogs. The high degree of similarity of the crystal packings of a homochiral crystal and racemic compounds, viz., the similar type of the homochiral hydrogen-bonded chains and analogous three-dimensional homochiral layers additionally stabilized by the interactions of the type C=O...C=O and C-H...O, allowed us to suggest the presence of the second, "missing" form for each sulfone. A directed search for the "missing" forms revealed the existence of the racemic modification of sulfone with the para-tolyl fragment formed during a very slow crystallization of the compound from benzene. No conglomerates of bromo and chloro analogs were found. Topological analysis of the electron density distribution performed by quantum chemical calculations using density functional theory (PBE1PBE, 6-31G(d,p)) showed the higher energy favorability of intermolecular interactions in the homochiral chains as compared to the hypothetical heterochiral associates. © 2013 Springer Science+Business Media New York.

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Keywords

2(5H)-furanones, crystallization, density functional theory (DFT), homochiral associates, intermolecular interactions, PBE1PBE functional, spontaneous resolution of enantiomers, sulfones, topological analysis, X-ray diffraction analysis