

Poster Presentation

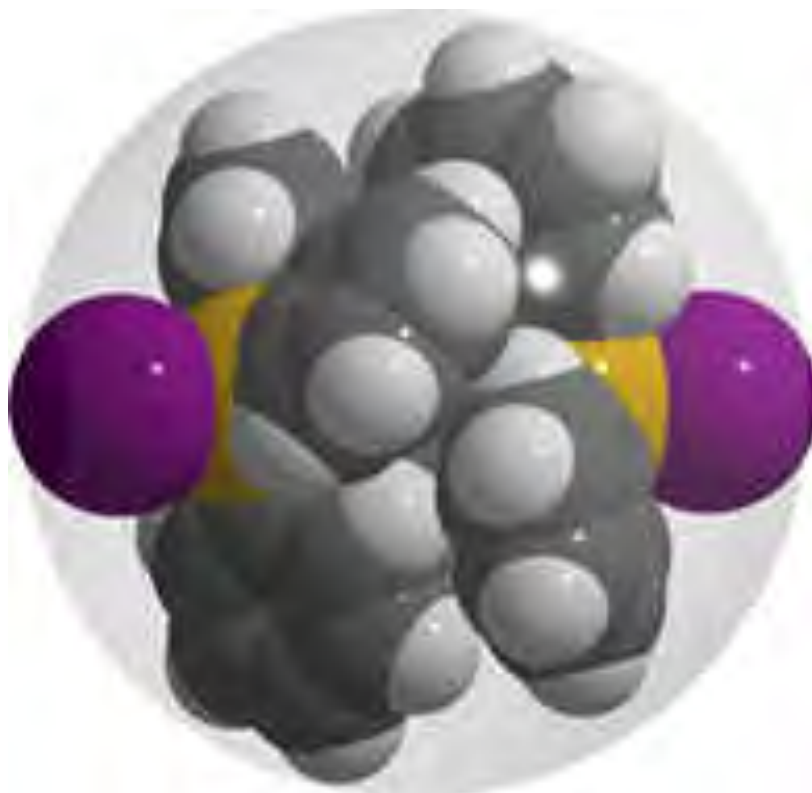
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New polymorphs of triphenyltin(IV) halides

H. Reuter¹, F. Ye¹, M. Reichelt¹, S. Schwidtko¹, J. Vages¹, S. Osthaar¹, A. Reuter¹, F. Mundt¹

¹University of Osnabrück, Institute of Chemistry of New Materials, Osnabrück, Germany

Triphenyltin(IV) halides, Ph_3SnHal with $\text{Hal} = \text{Cl}, \text{Br}, \text{and I}$, are white, low melting solids soluble in many indifferent organic solvents like chloroform or toluene. In these solutions as well as in solid they consist of isolated, tetrahedral molecules which intermolecular interactions restricted to van-der Waals ones. These molecules are characterized through the three aromatic phenyl rings attached at a certain pitch angle around the shaft of the tin-halide bond giving them a propeller-like shape accompanied by molecular chirality as the normal vectors of the blades can be oriented clock-wise or anti-clock-wise with respect to the tin-halide bond. In the past, a lot of different polymorphs of triphenyltin(IV) halides with up to 24 molecules in the unit cell have been described, all crystallizing in centrosymmetric space groups, implying that both chiral molecules are present. From a structural point of view there are still several questions of general interest: (i) how are both enantiomers distributed in these polymorphs, (ii) how are the molecular dipole moments arranged, and (iii) how are the different polymorphs related to each other. During various studies on the syntheses and reactivity of triphenyltin(IV) halides we found four additional polymorphs, which constitute new structure types in case of $\delta\text{-Ph}_3\text{SnI}$ ($Z = 8$, monoclinic, $P21/c$), and $\epsilon\text{-Ph}_3\text{SnI}$ ($Z = 12$, monoclinic, $P21/c$) or complete the already existing $\alpha\text{-Ph}_3\text{SnCl}$ structure type ($Z = 24$, rhomboedric, $R\bar{3}$) in case of $\beta\text{-Ph}_3\text{SnBr}$ and $\zeta\text{-Ph}_3\text{SnI}$. Analysing the new and already known polymorphs with respect to the three questions mentioned above points out (i) the influence of crystal symmetry elements (screw axes and glide planes) as well as (ii) the importance of the formation of supramolecular dimers composed of both enantiomers with an antiparallel orientation of the two molecular dipole moments, on the different structure types formed and their relation among each other.



Keywords: polymorphism, organotin(IV) compounds, supramolecular aggregates