

三苯基锡硫代苯甲酸酯的合成、性质和晶体结构

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摘要 用三苯基氯化锡与硫代苯甲酸在三乙胺存在下反应,合成了三苯基锡硫代苯甲酸酯,并进行了红外光谱及核磁共振氢谱表征。X射线单晶衍射表明,化合物属正交晶系,空间群P2₁2₁2₁,晶胞参数: a = 0.8306(3) nm, b = 1.6906(5) nm, c = 3.1459(10) nm, V = 4.417(2) nm³, Z = 8, D_c = 1.465 g/cm³, R₁ = 0.0472, wR₂ = 0.1012。该化合物的晶体是由孤立的分子所组成,四配位的锡原子呈畸变的四面体构型,配体羧基上的氧原子和锡原子之间存在弱的配位作用。

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[X射线衍射分析](#)

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Synthesis, Properties and Crystal Structure of Triphenyltin Thiobenzoate

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Abstract Triphenyltin thiobenzoate was synthesized by the reaction of triphenyltin chloride with thiobenzoic acid in the presence of Et₃N. The title complex was characterized by elemental analysis, IR and ¹H NMR spectra, and its crystal structure was determined by X-ray single crystal diffraction study. The crystal belongs to orthorhombic with space group P2₁2₁2₁, a = 0.8306(3) nm, b = 1.6906(5) nm, c = 3.1459(10) nm, V = 4.417(2) nm³, Z = 8, D_c = 1.465 g/cm³, R₁ = 0.0472, wR₂ = 0.1012. In the crystals, the structure consists of discrete molecule containing four-coordinate tin atom in a distorted tetrahedral configuration.

Key words [ORGANO TIN COMPOUNDS](#) [BENZENECARBOETHIOIC ACID](#) [CRYSTAL STRUCTURE](#) [TRIETHYL AMINE](#) [IR](#) [¹H NMR](#) [XRD](#)

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