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三(邻氯苄基)氯化锡的合成、结构和量子化学研究

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摘要　邻氯苄基氯与锡反应合成三(邻氯苄基)氯化锡，经x射线方法测定了新化合物 的晶体结构，化合物属三方晶系，空间群为R-3，晶体学参数：α=b=1．3583(4) mn，c=2．1147(8)am，v=3．3790(19)nm~3，Z=6，μ(Mo kα)=16．11cm~-1， r (000)：1572，R_1=O．0755；Sn-C键长分别为0．2148(13)和0．220(2)nm，Sn-C1 键为0．2528(15)和0．2477(13)Bill．中心锡原子与亚甲基碳和氯原子构成畸型四面体．并对其结构进行量子化学从头计算，探讨化合物的稳定性、分子轨道能量、原子净电荷布居规律以及一些前沿分子轨道的组成特征．

关键词　有机锡化合物　晶体结构　从头计算法　稳定性　分子轨道

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Study on Synthesis, Crystal Structure and Quantum Chemistry of the Tri(o-chlorobenzyl)tin Chloride

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Abstract　Abstract The re-butyl alcohol solution of o-chlorobenzyl chloride and Sn was heated to reflux for 5 h to yield the tri-(o-chlorobenzyl) tin chloride. The crystal and molecular structures of the compounds were determined by X-ray diffraction study. The crystal is trigonal system, space group R-3 with a = b = 1.3583(4) ran, c =2.1147(8) ran, V = 3.3790(19) ran~3, Z = 6, μ(Mo Ko) = 16.11 cm~(-1), F(OOO) = 1572, R_1=0.0755. The bond lengths of Sn- C1 are 0.2148 and 0.220 nm, respectively. The bond lengths of Sn-Cl are 0.2528 and 0.2477 ran, respectively. The tin atom has a distorted tetrahedral geometry. The study on tide compound has been performed with ah irutio calculation by means of G98W package and taking LanL2DZ basis set. The stabilities of the compound, some frontier molecular orbital energies, the populations of the atomic net charges in the molecule and the molecule characteristics of some frontier molecular orbitals have been discussed.

Key words　ORGANO TIN COMPOUNDS　CRYSTAL STRUCTURE　AB INITIO CALCULATION　STABILITY　MOLECULAR ORBIT

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