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Crystallographic report

The two-dimensional crystal structure of bis(trimethyltin)succinate, $[(Me_3Sn)_2(O_2CCH_2CH_2CO_2)]_\infty$

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A two-dimensional layer structure is found in the title compound comprising interconnected 22-membered rings and *trans*-C_3O_2 trigonal bipyramidal coordination geometries for tin. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; carboxylate; succinate; layer structure

COMMENT

The structural chemistry of the triorganotin carboxylates is rich and diverse.[1,2] For example, the structures of triorganotin dicarboxylates range from isolated dimeric,[3] to linear polymeric[3] to three-dimensional network structures.[4–6] In the title compound (Fig. 1), a new motif is found that features interconnected 22-membered rings. Each carboxylate ligand (disposed about a centre of inversion) is tetradentate and the tin atom geometry is *trans*-C_3O_2 trigonal bipyramidal.

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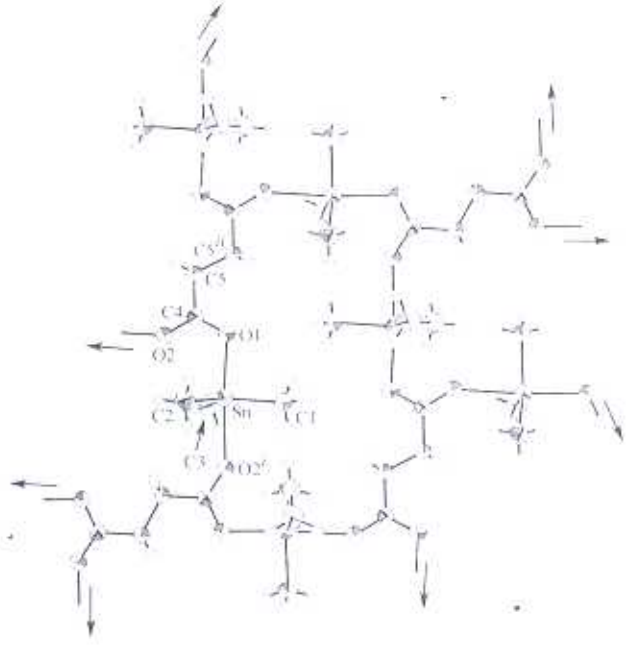

Figure 1. Two-dimensional structure of $[(Me_3Sn)_2(O_2CCH_2CH_2CO_2)]_\infty$. Key geometric parameters: Sn-O1 2.203(2), Sn-O2^{ii} 2.396(2), C4-O1 1.272(4), C4-O2 1.250(4), C5-C5^{i} 1.518(6) Å; O1-Sn-O2 175.99(8)°. Symmetry operations: *i* 1/2−*x*, 1/2 + *y*, 1/2 − *z*; *ii* −*x*, 2 − *y*, −*z*.

EXPERIMENTAL

The compound was prepared in 65% yield by adding a solution containing $(HO_2CCH_2)_2$ and two molar equivalents of Me_4NOH to an ethanol solution of Me_3SnCl (*warning: Me_3SnCl is highly toxic and must be used with due care*); m.p. 105–107 °C. Anal. (calc.) for $C_5H_{11}O_2Sn$: C, 26.46 (27.07); H, 4.85 (5.00); Sn, 52.65 (53.51). IR (cm^{-1}): 1584(s), 1427(m), 1409(m) ν(COO), 820(m) ν(C—C), 779(s) δ(COO), 677(m) ρ(COO), 553(m) ω(COO), 552(sh) $\nu_{as}(SnC_2)$, 287(sh) ν(Sn—O).^{1}H NMR, δ (ppm): 3.1 (s, 18H, CH_3), 4.35 (m, 4H, CH_2). ^{119}Sn NMR, δ (ppm)—248. Mössbauer data (mm s^{-1}): IS = 1.31, QS = 3.63, Γ = 0.79. Intensity data were collected at 293 K on a MAR345 image plate for a colourless block 0.12 × 0.20 × 0.20 mm^3. $C_5H_{11}O_2Sn$, M = 221.83, monoclinic, space group $C2/c$, a = 13.052(3), b = 9.460(4), c = 13.411(4) Å, β = 110.76(3)°, V = 1548.4(9) $Å^3$, Z = 8, 13 181 unique data (θ_{max} 27.5°), 1617 data with $I \geq 2\sigma(I)$, R = 0.052 (obs. data), wR = 0.122 (all data). Programs used: teXsan, SHELXL-97 and ORTEP. CCDC deposition number: 181234.

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