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Crystallographic report

6-Mercaptopurinate complex of tribenzyltin(IV), $(PhCH_2)_3Sn(C_5H_3N_4S)Sn(PhCH_2)_3OMe$

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The title complex displays a binuclear structure in which the geometries of tin atoms are different: one is cis-trigonal bipyramidal (with a C_3NS donor set) and the other is trans-trigonal bipyramidal (C_3NO). Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin(IV); 6-mercaptopurine

COMMENT

The structural chemistry of the triorganotin(IV) derivatives from heterocyclic thionates is rich and diverse.[1] For example, the structures of these compounds range from discrete[2] to trimeric[3] to polymeric.[4] In the title compound (Fig. 1), a novel structure is found that displays a binuclear structure as a result of the 6-mercaptopurinate anion being tridentate. The geometries of the tin atoms are different: one is cis-trigonal bipyramidal, the weak nature of the Sn···N interaction notwithstanding, and the other is trans-trigonal bipyramidal. The molecules are loosely associated via hydrogen-bonding interactions (N4···O1 = 2.87 Å) to form a chain.

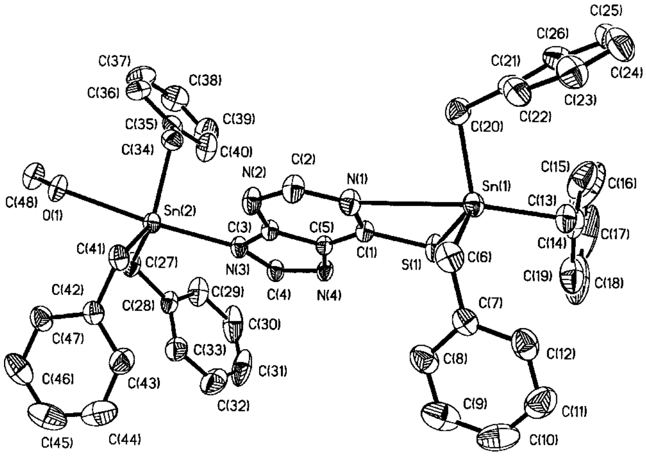

Figure 1. Molecular structure of $(PhCH_2)_3Sn(C_5H_3N_4S)Sn(PhCH_2)_3OMe$; hydrogen atoms have been removed for clarity. Selected geometric data: Sn1–S1 2.455(2), Sn1–N1 2.922(4), Sn2–O1 2.530(3), Sn2–N3 2.262(3) Å; S1–Sn1–N1 58.69(8), N1–Sn1–C13 157.00(12), O1–Sn2–N3 175.23(9)°.

EXPERIMENTAL

The reaction was carried out under an atmosphere of nitrogen using standard Schlenk techniques. 6-Mercaptopurine (0.152 g, 1 mmol) was added to a solution of methanol (20 ml) with sodium methoxide (0.054 g, 1 mmol), the mixture was stirred for 10 min, $(PhCH_2)_3SnCl$ (0.427 g, 1 mmol) was added, and the reaction mixture was stirred for 12 h at 40 °C. After cooling to room temperature and filtration, the solvent of the filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from methanol solution and pale-yellow crystals were formed; m.p. 158–160 °C. Anal. Found: C, 59.80; H, 5.15; N, 5.69. Calc. for $C_{48}H_{48}N_4OSSn_2$: C, 59.66; H, 5.01; N, 5.80%. IR (cm^{-1}): ν(C–S) 702, ν_{as}(Sn–C) 445, ν_s(Sn–C) 426, ν(Sn–S) 307. ^{1}H NMR: 8.20 (s, 1H, purine ring H^2), 7.98 (s, 1H, purine ring H^8), 6.89–7.16 (m, 30H, Sn–$CH_2C_6H_5$), 3.76 (s, 3H, Sn–OCH_3), 2.81 (s, 12H, Sn–$CH_2C_6H_5$). Intensity data were collected at 293(2) K on a Bruker SMART CCD 1000 diffractometer using a pale-yellow block 0.15 × 0.26 × 0.33 mm^3. $C_{48}H_{48}N_4OSSn_2$, $M = 966.34$, monoclinic, $P2_1/n$, $a = 10.857(11)$, $b = 28.10(3)$, $c = 14.989(15)$ Å, $\beta = 100.896(14)°$, $V = 4490(8)$ Å^3, $Z = 4$, 7857 unique data (θ_{max} 25.0°), $R = 0.033$ (5683 data with $I > 2\sigma(I)$), $wR = 0.070$ (all data). Software used: SHELXL-97 and ORTEP. CCDC deposition number: 227952.

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