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Crystallographic report

Bis[tri(*o*-chlorobenzyl)tin(IV)] piperazinylbisdithiocarbamate

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The centrosymmetric structure of $(o\text{-}C_6H_4CH_2)_3SnS_2CN(CH_2CH_2)_2NCS_2Sn(CH_2C_6H_4\text{-}o)_3$ features chelating dithiocarbamate ligands, so that a trigonal bipyramidal C_3S_2 coordination geometry for tin results. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; dithiocarbamate

COMMENT

The centrosymmetric dinuclear structure of $(o\text{-}C_6H_4CH_2)_3SnS_2CN(CH_2CH_2)_2NCS_2Sn(CH_2C_6H_4\text{-}o)_3$, Fig. 1, features chelating dithiocarbamate ligands that form unsymmetric Sn–S bonds. Each tin atom is five-coordinate within a C_3S_2 donor set that is best described as trigonal bipyramidal with the S2 and C18 atoms in axial positions. The structure is virtually identical to that of the Ph_3Sn analogue[1] and closely related to those of $(PhCH_2)_3S_2CNC_5H_{10}$[2] and $(PhCH_2)_3S_2CNC_4H_8O$;[3] the structural chemistry of tin 1,1-dithiolates has been summarized in reviews.[4,5]

EXPERIMENTAL

$NaS_2CN(CH_2CH_2)_2NCS_2Na\cdot H_2O$ (2.0 mmol) was added to a dichloromethane (30 ml) solution of tri(*o*-chlorobenzyl)tin(IV) chloride (4.0 mmol) and stirred for 10 h at 60 °C. The precipitated sodium chloride was removed by filtration and the filtrate was concentrated to about 5 ml under reduced pressure. Hexane (5 ml) was added to this solution and a precipitate was formed immediately. The product was recrystallized from a dichloromethane–hexane mixture. M.p.

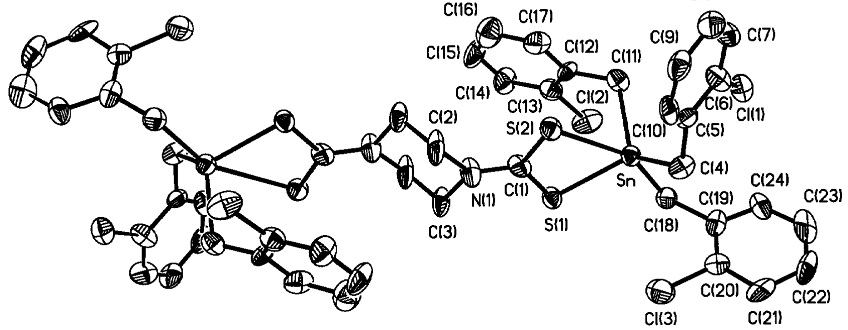

Figure 1. Molecular structure of $(o\text{-}C_6H_4CH_2)_3SnS_2CN(CH_2CH_2)_2NCS_2Sn(CH_2C_6H_4\text{-}o)_3$. Key geometric parameters: Sn–S(1) 2.435(4), Sn–S(2) 3.045(5), Sn–C(4) 2.220(10), Sn–C(11) 2.204(8), Sn–C(18) 2.180(9), S(1)–C(1) 1.706(9), S(2)–C(1) 1.664(10), N(1)–C(1) 1.319(11) Å; S(1)–Sn–S(2) 63.2(4), S(1)–Sn–C(4) 120.0(3), S(1)–Sn–C(11) 106.3(3), S(1)–Sn–C(18) 95.8(3), S(2)–Sn–C(4) 82.8(3), S(2)–Sn–C(11) 83.3(3), S(2)–Sn–C(18) 157.8(2), C(4)–Sn(1)–C(11) 117.5(4), C(4)–Sn–C(18) 103.4(4), C(11)–Sn–C(18) 111.4(3), S(1)–C(1)–S(2) 120.1(6)°.

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299–301 K. IR (KBr): ν(C–N) 1489, ν(C–S) 998 cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a colorless block $0.10 \times 0.15 \times 0.20$ mm^3. $C_{48}H_{44}Cl_6N_2S_4Sn_2$, $M = 1227.17$, monoclinic, $P2_1/c$, $a = 10.33(2)$, $b = 25.69(5)$, $c = 10.33(2)$ Å, $\beta = 115.22(3)°$, $V = 2478(8)$ Å^3, $Z = 2$, 3891 unique data ($\theta_{max} = 25.2°$), 1759 data with $I > 2\sigma(I)$. $R = 0.065$ (obs. data), $wR = 0.108$ (all data); $\rho_{max} = 0.81$ e$^-$ Å^{-3}. Program used: SHELXL and ORTEP. CCDC deposition number: 224294.

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