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Crystallographic report

Chlorodi(*o*-chlorobenzyl)tin *N*-methylpiperazinyldithiocarbamate

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The tin atom in (2-*Cl*-$C_6H_4CH_2)_2Sn(Cl)S_2CN(CH_2CH_2)_2NCH_3$ is in a trigonal bipyramid geometry defined by a C_2ClS_2 donor set with the chlorine and weakly bound sulfur atoms in axial positions.

KEYWORDS: crystal structure; organotin; dithiocarbamate

COMMENT

A trigonal bipyramidal geometry about the tin atom (Fig. 1) was found in (2-*Cl*-$C_6H_4CH_2)_2Sn(Cl)S_2CN(CH_2CH_2)_2NCH_3$ that was investigated during the study of the structural diversity in these and analogous organotin dithiocarbamates.[1–5] The structure is similar, for example, to those reported for $(PhCH_2)_2SnCl(S_2CNC_5H_{10})$[3] and $(PhCH_2)_2SnCl(S_2CNC_4H_8O)$.[4]

EXPERIMENTAL

The Na[*N*-methylpiperazinyldithiocarbamate] (1.0 mmol) was added to a CH_2Cl_2 solution (30 ml) of di(*o*-chlorobenzyl)tin dichloride (1.0 mmol) and stirred for 8 h at 30 °C. The precipitated NaCl 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 immediately a precipitate was formed. The product was recrystallized from CH_2Cl_2–hexane to give colorless crystals; m.p. 114–115 °C. IR (KBr), ν: 1481, 1134, 1001, 557, 462 cm^{-1}. Intensity data were collected at 273 K on a Bruker Smart 1000 CCD for a block $0.35 \times 0.43 \times 0.49$ mm^3. $C_{20}H_{23}Cl_3N_2S_2Sn$, $M = 580.56$, monoclinic, $P2_1/n$, $a = 15.944(7)$, $b = 8.188(4)$, $c = 18.888(8)$ Å, $\beta = 95.728(6)°$, $V = 2453.6(18)$ $Å^3$, $Z = 4$, 4325 unique data ($\theta_{max} = 25.0°$), $R = 0.028$ (3281 data with $I \geq 2\sigma(I)$), $wR = 0.086$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 240374.

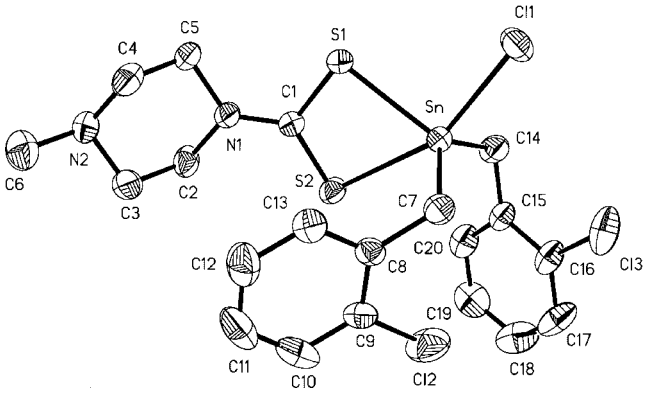

Figure 1. The molecular structure of (2-*Cl*-$C_6H_4CH_2)_2Sn(Cl)S_2CN(CH_2CH_2)_2NCH_3$; hydrogen atoms omitted for clarity. Key geometric parameters: Sn–Cl1 2.4706(14), Sn–S1 2.4668(14), Sn–S2 2.6981(14), Sn–C7 2.149(4), Sn–C14 2.163(4) Å; Cl1–Sn–S1 88.74(4), Cl1–Sn–S2 156.66(4), Cl1–Sn–C7 96.97(10), Cl1–Sn–C14 94.98(12), S1–Sn–S2 69.54(3), S1–Sn–C7 106.76(11), S1–Sn–C14 123.18(11), S2–Sn–C7 97.41(10), S2–Sn–C14 92.22(12), C7–Sn–C14 128.75(15)°.

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