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Crystallographic report

Di(*p*-chlorobenzyl)tin bis(*N*-methylpiperazinyldithiocarbamate)

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The tin atom in (4-*Cl*-$C_6H_4CH_2)_2Sn[S_2CN(CH_2CH_2)_2NCH_3]_2$ is in a C_2S_4 skew-trapezoidal bipyramidal geometry with the two carbon atoms being disposed over the weaker Sn–S bonds.

KEYWORDS: crystal structure; di(*p*-chlorobenzyl)tin; *N*-methylpiperazinyldithiocarbamate

COMMENT

A skew-trapezoidal bipyramidal geometry about the tin atom was found in the title structure, Fig. 1, as is usually found in structures of this type,[1,2] for example in the related benzyl derivatives: $(PhCH_2)_2Sn(S_2CNC_5H_{10})_2$[3] and $(PhCH_2)_2Sn(S_2CNC_4H_8O)_2$.[4]

EXPERIMENTAL

The sodium salt of *N*-methylpiperazinyldithiocarbamate (4.0 mmol) was added to a dichloromethane solution (30 ml) of di(*p*-chlorobenzyl)tin dichloride (2.0 mmol) and stirred for 14 h at 30 °C. The filtrate was concentrated to about 5 ml under reduced pressure. Hexane (5 ml) was added to this solution; immediately a precipitate was formed which was recrystallized from dichloromethane–hexane to give colorless crystals; m.p. 201–203 °C, IR (KBr), ν 1485, 1143, 1011, 541, 446 cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block $0.27 \times 0.35 \times 0.41$ mm^3. $C_{26}H_{34}Cl_2N_4S_4Sn$, $M = 720.40$, monoclinic, $P2_1/c$, $a = 13.8624(12)$, $b = 12.554(4)$, $c = 19.711(5)$ Å, $\beta = 109.992(5)°$, $V = 3223.5(14)$ $Å^3$, $Z = 4$, 5677 unique data ($\theta_{max} = 25.0°$), $R = 0.042$ [3341 data with $I > 2\sigma(I)$], $w = 0.112$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition no. 235735.

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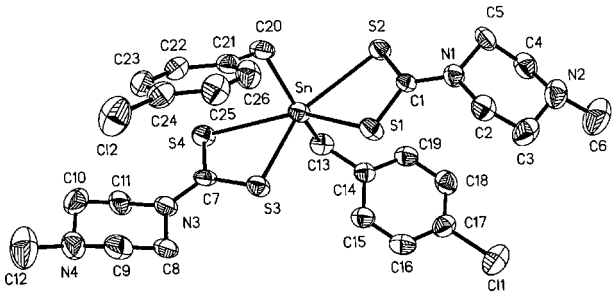

Figure 1. The molecular structure of (4-*Cl*-$C_6H_4CH_2)_2Sn[S_2CN(CH_2CH_2)_2NCH_3]_2$; H atoms are omitted. Key geometric parameters: Sn–S1 2.5495(14), Sn–S2 2.8575(14), Sn–S3 2.5338(14), Sn–S4 2.9683(15) Å; S1–Sn–S2 65.91(4), S1–Sn–S3 84.80(5), S1–Sn–S4 149.49(4), S2–Sn–S3 150.61(4), S2–Sn–S4 144.60(4), S3–Sn–S4 64.73(4), C13–Sn–C20 146.9(2)°.

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