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Crystallographic report

Di(*o*-chlorobenzyl)tin(IV) bis(*N*-methylpiperazinyldithiocarbamate)

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The tin atom in $\{(2\text{-}Cl\text{-}C_6H_4CH_2)_2Sn[S_2CN(CH_2CH_2)_2NCH_3]_2\}_2$ is in a skew-trapezoidal bipyramidal geometry defined by a C_2S_4 set with C–Sn–C 150.61(19)°. Centrosymmetric pairs associated via weak Sn···S to form a dimer. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; dithiocarbamate

COMMENT

The structural chemistry of organotin dithiocarbamates is both rich and diverse, so that monomeric, dimeric, and one-dimensional chain structures are known.[1–6] In the title structure (Fig. 1), the tin atom exists in skew-trapezoidal bipyramidal geometry and weakly bridged centrosymmetric dimers are found with Sn···S3^{i} of 3.9071(12) Å.

EXPERIMENTAL

Na[*N*-methylpiperazinyldithiocarbamate] (2.0 mmol) was added to a CH_2Cl_2 solution (30 ml) of di(*o*-chlorobenzyl)tin dichloride (1.0 mmol) and stirred for 16 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. 147–148 °C. IR (KBr), ν: 1481, 1140, 1001, 545, 442 cm^{-1}. Intensity data were collected at 273 K on a Bruker Smart 1000 CCD for a block 0.31 × 0.36 × 0.47 mm^3. $C_{26}H_{34}Cl_2N_4S_4Sn$, $M = 720.40$, monoclinic, $P2_1/n$, $a = 9.1174(12)$, $b = 24.958(3)$, $c = 13.9422(18)$ Å, $\beta = 104.088(2)°$, $V = 3077.2(7)$ Å^3, $Z = 4$, 5424 unique data ($\theta_{max} = 25.0°$), $R = 0.039$ (3927 data with $I \geq 2\sigma(I)$), $wR = 0.105$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 245406.

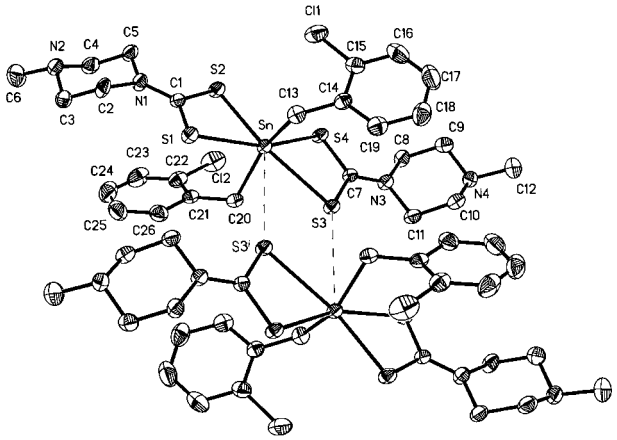

Figure 1. The molecular structure of $\{(2\text{-}Cl\text{-}C_6H_4CH_2)_2Sn[S_2CN(CH_2CH_2)_2NCH_3]_2\}_2$; hydrogen atoms are omitted for clarity. Key geometric parameters: Sn–S1 2.8049(13), Sn–S2 2.5401(13), Sn–S3 2.8674(12), Sn–S4 2.5676(12), Sn–C13 2.184(5), Sn–C20 2.184(5) Å; S1–Sn–S2 67.49(4), S1–Sn–S3 131.37(4), S1–Sn–S4 162.38(4), S2–Sn–S3 160.79(4), S2–Sn–S4, 95.33(4), S3–Sn–S4 66.07(3), C13–Sn–C20 150.61(19)°.

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