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Crystallographic report

Dibenzyltin(IV) bis(*N*,*N*-dibenzyldithiocarbamate)

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A distorted octahedron C_2S_4 geometry is found for the tin atom in the title compound; C–Sn–C is 136.61(19)°. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; dibenzyltin; *N*,*N*-dibenzyldithiocarbamate

COMMENT

A distorted octahedron geometry about the tin atom was found in the title structure that was investigated during the study of the structural diversity in these and analogous organotin dithiocarbamates (Fig. 1).[1–3] The structure is similar, for example, to those reported for the compounds $(PhCH_2)_2Sn(S_2CNEt_2)_2$,[4] $(PhCH_2)_2Sn(S_2CNC_4H_8)_2$,[4] and $(PhCH_2)_2Sn(S_2CNC_4H_8O)_2$.[5]

EXPERIMENTAL

Sodium *N*,*N*-dibenzyldithiocarbamate (2.0 mmol) was added to a CH_2Cl_2 solution (30 mL) of $(PhCH_2)_2SnCl_2$ (1.0 mmol) and stirred for 12 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) were added to this solution and immediately a precipitate was formed. The product was recrystallized from CH_2CH_2–hexane to give colorless crystals; m.p. 145–147 °C; IR (KBr), ν: 1468, 1140, 995, 542, 454 cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block $0.33 \times 0.41 \times 0.46$ mm^3. $C_{44}H_{42}N_2S_4Sn$, $M = 845.73$, monoclinic, $P2_1/n$, $a = 9.990(8)$, $b = 39.09(3)$, $c = 11.122(9)$ Å, $\beta = 111.370(10)°$, $V = 4045(6)$ $Å^3$, $Z = 4$, 6905 unique data ($\theta_{max} = 25.0°$), $R = 0.060$ (5636 data with $I > 2\sigma(I)$), $wR = 0.094$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 232636.

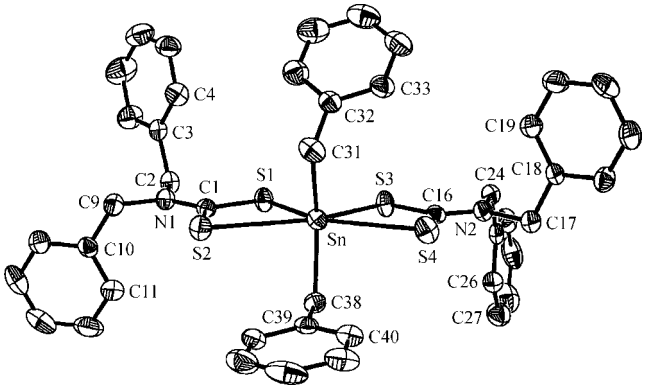

Figure 1. The molecular structure of $(PhCH_2)_2Sn[S_2CN(CH_2Ph)_2]_2$; hydrogen atoms have been omitted for clarity. Key geometric parameters: Sn–S1 2.521(2), Sn–S2 3.004(2), Sn–S3 2.521(2), Sn–S4 2.942(2), Sn–C31 2.154(5), Sn–C38 2.155(5) Å; S1–Sn–S3 81.17(6), S2–Sn–S4 149.59(5), C31–Sn–C38 136.61(19)°.

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