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Crystallographic report

Di(*p*-fluorobenzyl)tin bis(*N*,*N*-dimethyldithiocarbamate)

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The tin atom in $(p\text{–}FC_6H_4CH_2)_2(S_2CNMe)_2$ is in a skewed-trapezoidal bipyramidal geometry defined by two sets of sulfur donors derived from the dithiocarbamate ligands and two carbon atoms from the tin-bound *p*-fluorobenzyl substituents; C–Sn–C is 129.2(2)°.

KEYWORDS: crystal structure; di(*p*-fluorobenzyl)tin; dithiocarbamate

COMMENT

In the title compound, $(p\text{-}FC_6H_4CH_2)_2(S_2CNMe)_2$, Fig. 1, the dithiocarbamate ligands form asymmetric Sn–S bond distances, so that a skewed-trapezoidal bipyramidal geometry about the tin atom results in which the organo substituents are disposed over the weaker Sn–S bonds. This result is in accord with the literature structures of the general formula $R_2Sn(S_2CNR'_2)_2$.[1–6]

EXPERIMENTAL

The anhydrous sodium salt of dimethyldithiocarbamate (2.0 mmol) was added to a dichloromethane solution (30 ml) of di(*p*-fluorobenzyl)tin dichloride (1.0 mmol) and stirred for 10 h at 30 °C. The NaCl precipitated 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 dichloromethane–ethyl ether to give colorless crystals. M.p. 138–139 °C; IR (KBr): ν 1488 (C–N), 1001 (C–S), 545 (Sn–C), 452 (Sn–C) cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block $0.05 \times 0.25 \times 0.90$ mm^3. $C_{20}H_{24}F_2N_2S_4Sn$, $M = 577.34$, triclinic, $P\bar{1}$, $a = 7.400(4)$, $b = 13.009(7)$, $c = 13.858(7)$ Å, $\alpha = 69.623(7)$, $\beta = 76.193(6)$, $\gamma = 77.453(7)°$, $V = 1201.3(10)$ $Å^3$, $Z = 2$, 4194 unique data ($\theta_{max} = 25.0°$), $R = 0.039$ (3141 data with $I \geq 2\sigma(I)$), $wR = 0.125$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 231733.

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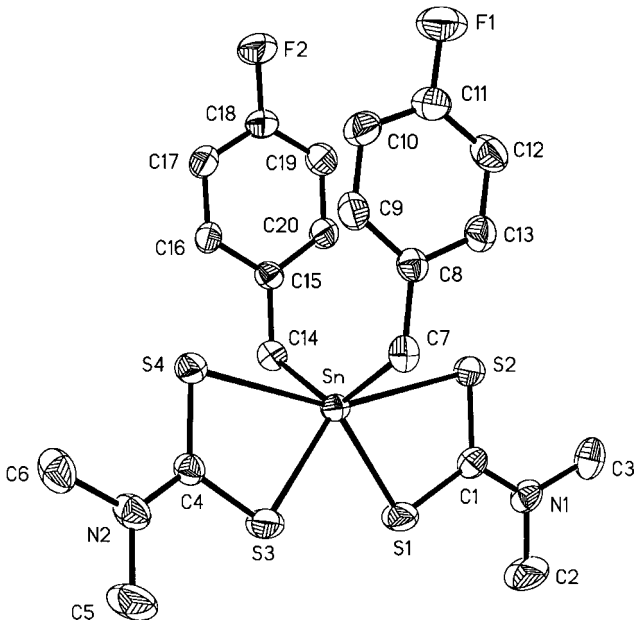

Figure 1. The molecular structure of $(p\text{-}FC_6H_4CH_2)_2(S_2CNMe)_2$; hydrogen atoms are omitted. Key geometric parameters: Sn–S1 2.5257(19), Sn–S2 2.9532(19), Sn–S3 2.5186(19), Sn–S4 3.0020(18), Sn–C7 2.157(6), Sn–C14 2.167(6) Å; S1–Sn–S2 64.50(6), S1–Sn–S3, 78.32(6), S1–Sn–S4 141.42(5), S2–Sn–S3 141.27(6), S2–Sn–S4 154.08(5), S3–Sn–S4 63.84(5), C7–Sn–C14 129.2(2)°.

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