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Crystallographic report

Dibenzyl(dichloro)(1,10-phenanthroline)tin (IV) chloroform solvate

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The monomeric title compound features a distorted octahedral tin (IV) centre within a $C_2Cl_2N_2$ donor set with two *cis* Cl atoms and two *trans* benzyl groups. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; 1,10-phenanthroline

COMMENT

The monomeric distorted octahedral tin (IV), which crystallizes as a chloroform solvate (Fig. 1), has two *cis* chlorides and two *trans* benzyl groups. The non-centrosymmetric structure exhibits an Sn–Cl–$HCCl_3$ interaction of 2.51 Å, leading to the elongation of the Sn–Cl1 bond by 0.1 Å; this is responsible for the deviation from 2-fold symmetry. This structure is a pseudo-polymorphic modification of the reported unsolvated complex in which the Sn–Cl bond lengths are experimentally equivalent.[1]

EXPERIMENTAL

The $(PhCH_2)_2SnCl_2$(phen) compound was prepared by the reaction of 1,10-phenanthroline and dibenzyltin chloride[2] in methanol solution. Analytically pure crystals of diffraction quality were obtained by recrystallization of the product from chloroform solution. Yield was 72%, m.p. 210–211 °C and ^{119}Sn NMR (δ) −337.8 ppm. Intensity data were collected at 293 K on an Enraf-Nonius CAD-4 diffractometer for a colourless block $0.20 \times 0.25 \times 0.30$ mm^3. $C_{26}H_{22}Cl_2N_2Sn{\cdot}CHCl_3$, $M = 671.41$, monoclinic, Cc, $a = 18.594(8)$, $b = 10.558(3)$, $c = 15.892(9)$ Å, $\beta = 114.82(4)°$, $V = 2832(2)$ Å^3, $Z = 4$, $R = 0.059$ [2325 data with $I \geq 2\sigma(I)$, $\theta_{max} = 25.0$], $wR = 0.153$ (all 2581 data), $\rho_{max} = 2.15$ (near Sn) eÅ^{-3}. Programs used: WINGX, SIR92, SHELXL and ORTEP. CCDC deposition no. 235 283.

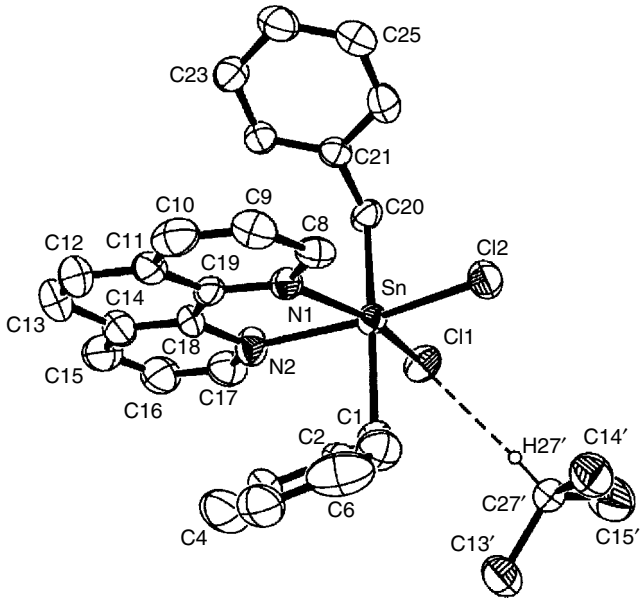

Figure 1. Molecular structure of $(PhCH_2)_2SnCl_2$(phen)·$CHCl_3$. Key geometric parameters: Sn-Cl1 2.594(3), Sn-Cl2 2.493(4), Sn-N1 2.338(8), Sn-N2 2.334(13) Å; C1-Sn-C20 170.6(6), Cl1-Sn-Cl2 105.24(12), N1-Sn-N2 69.4(4)° (symmetry code′ = $x + 1/2, y + 1/2, z$).

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