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Crystallographic report

1,4-Bis(triphenylstannylmethyldimethylsilyl)benzene, *p*-$(Ph_3SnCH_2SiMe_2)_2C_6H_4$

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The dinuclear molecule of *p*-$(Ph_3SnCH_2SiMe_2)_2C_6H_4$ adopts an 'S' conformation in the solid state, which is stabilized by C—H···π interactions. Distorted tetrahedra defined by C_4 donor sets are found for the tin atoms. Copyright © 2002 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; C—H···π interactions

COMMENT

The title compound, *p*-$(Ph_3SnCH_2SiMe_2)_2C_6H_4$ (**I**),[1] is a synthetic precursor to spacer-linked tetraorganodistannoxanes. The structure of **I** (Fig. 1) shows an 'S' conformation that is stabilized, in part, by an intramolecular C—H···π interaction.[2] In this way, the C32-*H* atom is directed towards the ring centroid of C22—C27 so that the distance separating them is 2.89 Å and the angle subtended at H is 172°. The molecule features distorted tetrahedral tin centres defined by C_4 donor sets. The Sn—C bond distances lie in the range 2.115(6) to 2.145(6) Å and the C—Sn—C angles are in the range 105.0(2) to 117.4(2)°. The widest of these angles involve the tin-bound methylene groups.

EXPERIMENTAL

Crystallography

Intensity data for **I** were collected at 293 K on a Rigaku AFC6R diffractometer for a colourless crystal $0.11 \times 0.24 \times 0.32$ mm^3. $C_{48}H_{50}Si_2Sn_2$, $M = 920.5$, triclinic, $P\bar{1}$, $a = 13.393(5)$, $b = 14.366(4)$, $c = 11.990(4)$ Å, $\alpha = 91.14(3)$, $\beta = 105.20(3)$, $\gamma = 98.43(3)°$, $V = 2198(1)$ Å^3, $Z = 2$, 10165 unique data (θ_{max} 27.5°), 5336 data with $I \geq 3\sigma(I)$, R(obs.) = 0.042, wR(obs.) = 0.044, $\rho_{max} = 0.71$ e$^-$ Å^{-3}. Programs used: teXsan, DIRDIF, DIFABS, PLATON, and ORTEP. CCDC deposition number: 138683.

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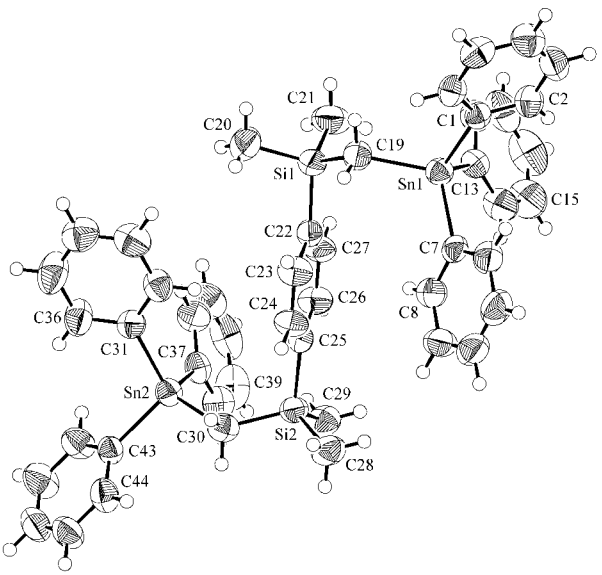

Figure 1. Molecular structure of (**I**).