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Triphenyltetradecylstannane

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In the title compound, $[Sn(C_{14}H_{29})(C_6H_5)_3]$, the coordination around the Sn atom is distorted tetrahedral, with the Sn—C bonds being in the range 2.136 (2)–2.155 (2) Å and the C—Sn—C angles being in the range 107.22 (9)–113.16 (10)°.

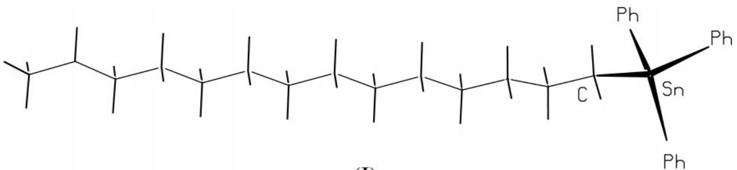
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.071
Data-to-parameter ratio = 21.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In the title compound, (I), the coordination around the Sn atom is distorted tetrahedral, with the Sn—C bonds being in the range 2.136 (2)–2.155 (2) Å and the C—Sn—C angles being in the range 107.22 (9)–113.16 (10)°. Full details of the Sn connectivity is given in Table 1. A view of the molecule is shown in Fig. 1.



(I)

Examination of the structure with *PLATON* (Spek, 2000) showed that there were no solvent-accessible voids in the crystal lattice.

Experimental

The title compound was prepared from Ph_3SnCl and $CH_3(CH_2)_{13}MgBr$ in thf, was purified by column chromatography on silica, using petroleum ether as eluent and was recrystallized from EtOH. M.p. 334–336 K.

Crystal data

$[Sn(C_{14}H_{29})(C_6H_5)_3]$
M_r = 547.36
Triclinic, $P\overline{1}$
a = 7.5468 (15) Å
b = 9.874 (2) Å
c = 20.378 (4) Å
α = 95.20 (3)°
β = 91.64 (3)°
γ = 110.15 (3)°
V = 1416.8 (5) Å^3
Z = 2
D_x = 1.283 Mg m^{-3}
Mo Kα radiation
Cell parameters from 15659 reflections
θ = 3.0–27.5°
μ = 0.92 mm^{-1}
T = 150 (1) K
Plate, colourless
0.55 × 0.10 × 0.01 mm

Data collection

KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.632, T_{max} = 0.991
21 212 measured reflections
6331 independent reflections
5073 reflections with$I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -26 \rightarrow 26$

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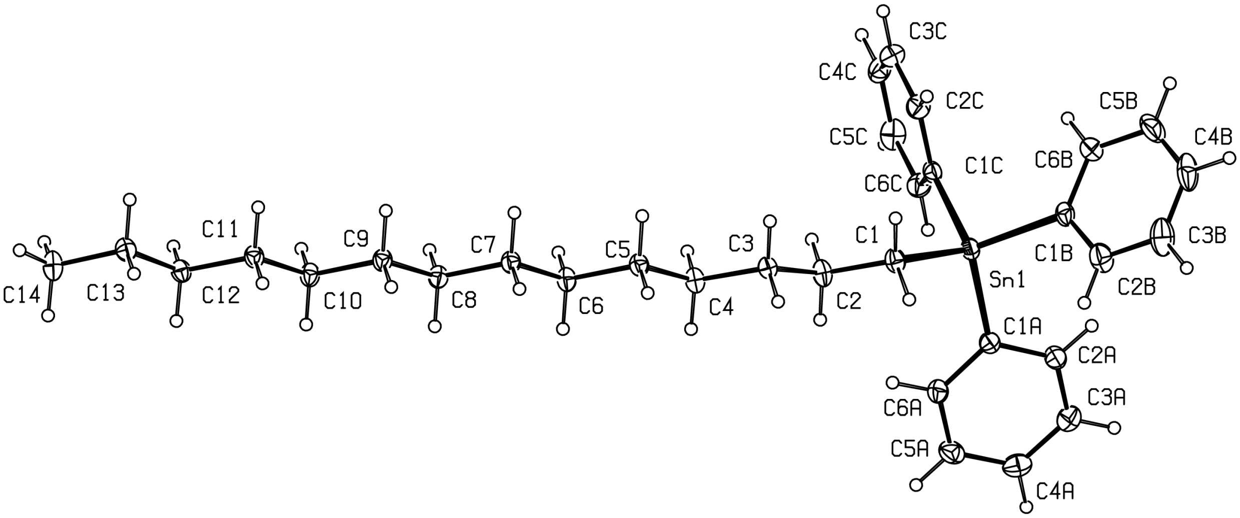

Figure 1
A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

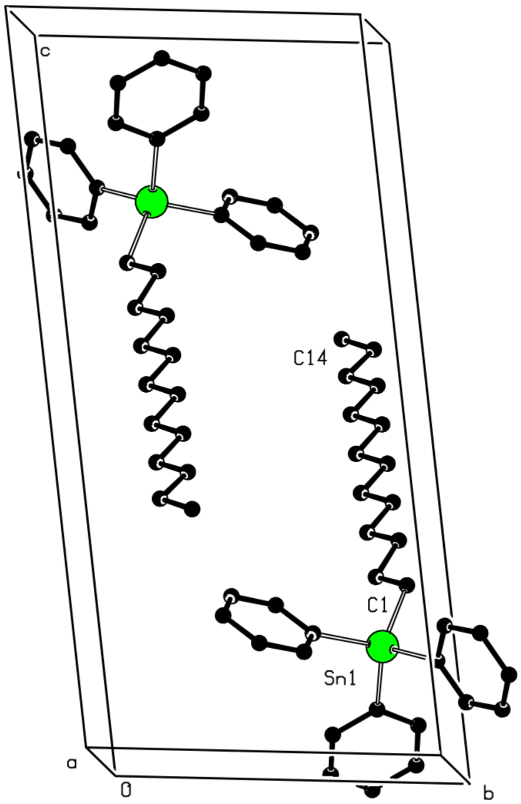

Figure 2
A view of the crystal structure.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.071$
$S = 1.00$
6331 reflections
298 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0310P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.84$ e Å^{-3}
$\Delta\rho_{\min} = -0.77$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1*C*	2.136 (2)	Sn1—C1*A*	2.142 (2)
Sn1—C1*B*	2.141 (3)	Sn1—C1	2.155 (2)
C1*C*—Sn1—C1*B*	109.13 (10)	C1*C*—Sn1—C1	107.22 (9)
C1*C*—Sn1—C1*A*	110.14 (9)	C1*B*—Sn1—C1	108.63 (9)
C1*B*—Sn1—C1*A*	108.48 (9)	C1*A*—Sn1—C1	113.16 (10)

H atoms were treated as riding with C—H distances in the range 0.95–0.99 Å.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton, using an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice.

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