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(2-Methyl-2-phenylpropyl)triphenylstannane

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.067
Data-to-parameter ratio = 13.4

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

Bond lengths and angles in the title compound, $[Sn(C_6H_5)_3(C_{10}H_{13})]$, are as expected for a molecule of this kind. The packing of the molecules in well defined layers results in a number of C—H$\cdots\pi$ intermolecular contacts.

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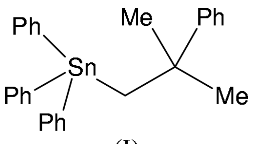
Comment

One component of the title compound, (I), is the 2-methyl-2-phenylpropyl or neophyl group (neo). The compound may therefore be formulated as (neo)Ph_3Sn. Fig. 1 is a drawing of the molecule, and distances and angles involving Sn are given in Table 1. These, along with benzene ring C—C distances and internal C—C—C angles, and distances and angles involving alkyl C atoms of the neophyl group [1.363 (6)–1.400 (5) Å and 117.2 (3)–121.2 (3)°, and 1.524 (4)–1.536 (5) Å and 106.3 (3)–112.0 (3)°, respectively], are unremarkable for a compound of this kind. However, two notable features are present in the structure. The first of these concerns the disposition within the molecule of the phenyl groups bonded directly to the Sn atom. For convenience in what follows, the four phenyl groups present in the molecule are designated as Ph1 with ring centroid *Cg*1, comprising atoms C5–C10, Ph2 with centroid *Cg*2, comprising C11–C16, Ph3 with centroid *Cg*3, comprising C17–C22, and Ph4 with centroid *Cg*4, comprising C23–C28. As is clearly shown in Fig. 1, Ph1 is part of the neophyl group and Ph2–Ph4 are the phenyl groups directly bonded to Sn. Ph2–Ph4 adopt the propeller-shaped configuration relative to Sn that is characteristic of the Ph_3Sn moiety, but the dihedral angles between their least-squares planes cover the unusually wide range of 49.55 (11)–87.13 (12)°. The values for the displacements of selected atoms from the plane defined by C11, C17 and C23 (see deposited CIF for details) confirm the propeller-shaped configuration but show that Ph2 has the greatest tilt relative to the reference plane and Ph3 the least. This configuration is attributed to the need to accommodate the steric requirements of the neophyl substituent.



(I)

The second notable feature of this structure is the manner in which the molecules are packed in layers (Fig. 2) parallel to (010), *b*/2 thick and centred on $y = 0$ and $\frac{1}{2}$. This arrangement, with phenyl groups directly attached to Sn on the surfaces of the layers, favours a number of C—H$\cdots\pi$ intermolecular contacts, as given in Table 2 and shown, in part, in Fig. 2. The

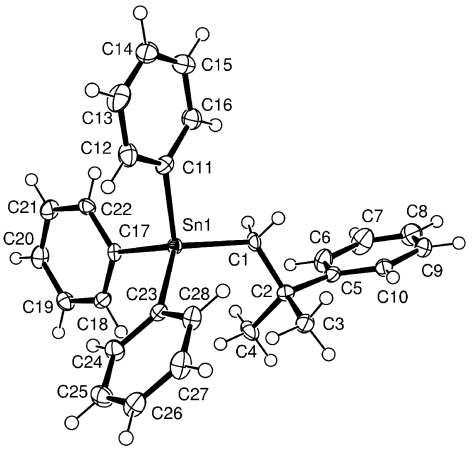


Figure 1

The molecule of (I). Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii.

contacts shown in Fig. 2 are those that occur within the layers of molecules. The contact present in Table 2 that is not shown in Fig. 2 is the interlayer contact C14—H14$\cdots$*Cg*4$^{\rm vii}$. The H$\cdots$*Cg* distances are all greater than 2.98 Å and the significance of these interactions in terms of the formation of even very weak bonds, as distinct from simple packing requirements, remains doubtful, although they can be regarded as electrostatic interactions.

Experimental

Compound (I) was obtained from the Grignard reaction of neophyl magnesium bromide, neoMgBr, prepared from neoBr (10.7 g, 0.05 mol) and Mg (0.18 g, 0.075 mol) in tetrahydrofuran (50 ml) with Ph_3SnCl (14.5 g, 0.038 mol). Crystals suitable for analysis (m.p. 367–368 K) were obtained by recrystallization from ethanol. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.48 (*s*, 6H, Me), 2.18 [*s*, 2H, $J(^{119,117}$Sn–^{1}H) = 56.1 Hz, CH_2Sn], 7.1–7.2 (*m*, 5H, Ph_{neo}), 7.3–7.5 (*m*, 15H, PhSn). ^{13}C NMR (100 MHz, $CDCl_3$): δ 31.9 [$J(^{119,117}$Sn–^{13}C) = 392, 376 Hz, CH_2], 33.1 [$J(^{119,117}$Sn–^{13}C) = 64.8 Hz, CMe_2], 38.1 [$J(^{119,117}$Sn–^{13}C) = 18.2 Hz, Me], 125.3 (C_m, Ph_{neo}), 125.7 (C_p, Ph_{neo}), 128.2 (C_o, Ph_{neo}), 128.3 [$J(^{119,117}$Sn–^{13}C) = 48.6 Hz, C_m, PhSn], 128.5 [$J(^{119,117}$Sn–^{13}C) = 10.6 Hz, C_p, PhSn], 136.9 [$J(^{119,117}$Sn–^{13}C) = 35 Hz, C_o, PhSn], 139.8 [$J(^{119,117}$Sn–^{13}C) = 483 and 461 Hz, C_{ipso}, PhSn], 150.1 (C_{ipso}, Ph_{neo}). ^{119}Sn NMR (93 MHz, $CDCl_3$): δ −115.6.

Crystal data

$[Sn(C_6H_5)_3(C_{10}H_{13})]$
M_r = 483.19
Orthorhombic, *Aba*2
a = 22.8724 (5) Å
b = 17.0573 (4) Å
c = 11.6326 (3) Å
V = 4538.36 (19) Å^3
Z = 8
D_x = 1.414 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 4339 reflections
θ = 2.9–27.5°
μ = 1.14 mm^{-1}
T = 120 (2) K
Block, colourless
0.60 × 0.35 × 0.30 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.556, T_{max} = 0.711
7972 measured reflections

3545 independent reflections
3358 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°
h = −26 → 29
k = −18 → 22
l = −10 → 14

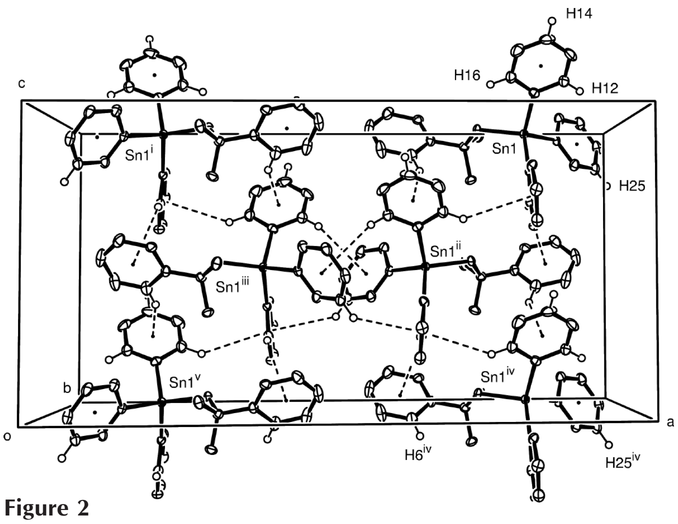


Figure 2

Molecules of (I) in a layer parallel to (010) and centred on *x* = 1. Dashed lines indicate C—H$\cdots\pi$ contacts. Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii. Selected atoms are labelled. [Symmetry codes: (i) $1 - x, 2 - y, z$; (ii) $\frac{3}{2} - x, y, z - \frac{1}{2}$; (iii) $x - \frac{1}{2}, 2 - y, z - \frac{1}{2}$; (iv) $x, y, z - 1$; (v) $1 - x, 2 - y, z - 1$.]

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.067$
S = 1.08
3545 reflections
265 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 2.271P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00349 (14)
Absolute structure: Flack (1983), 887 Friedel pairs
Flack parameter = 0.04 (3)

Table 1

Selected geometric parameters (Å, °).

Sn1—C11	2.139 (4)	Sn1—C17	2.145 (4)
Sn1—C23	2.142 (3)	Sn1—C1	2.163 (3)
C11—Sn1—C23	109.53 (15)	C23—Sn1—C1	118.93 (11)
C11—Sn1—C17	106.97 (11)	C17—Sn1—C1	109.10 (13)
C23—Sn1—C17	107.73 (15)	C2—C1—Sn1	121.1 (2)
C11—Sn1—C1	103.98 (15)		

Table 2

Distances and angles (Å, °) associated with intermolecular C—H$\cdots\pi$ contacts in (I).

C—H$\cdots$*Cg*^{a}	H$\cdots$*Cg*	$H_{perp}{}^b$	γ^c	C—H$\cdots$*Cg*	C$\cdots$*Cg*
C6—H6$\cdots$*Cg*2$^{\rm ii}$	3.10	3.03	12	143	3.90
C12—H12$\cdots$*Cg*4$^{\rm vi}$	3.21	3.02	20	127	3.86
C14—H14$\cdots$*Cg*4$^{\rm vii}$	3.19	3.08	15	144	4.00
C16—H16$\cdots$*Cg*3$^{\rm viii}$	3.18	3.05	16	140	3.95
C18—H18$\cdots$*Cg*1$^{\rm ii}$	3.24	3.13	14	133	3.94
C25—H25$\cdots$*Cg*3$^{\rm vi}$	2.98	2.95	8	137	3.74

Notes: (*a*) *Cg*1–*Cg*4 are, respectively, the centroids of the rings defined byC5–C10, C11–C16, C17–C22 and C23–C28; (*b*) H_{perp} is the perpendicular distance of H from the π-acceptor ring; (*c*) γ is the angle at H between H$\cdots$*Cg* and H_{perp}. Symmetry codes: (ii) $\frac{3}{2} - x, y, z - \frac{1}{2}$; (vi) $2 - x, 2 - y, z$; (vii) $x, y - \frac{1}{2}, \frac{1}{2} + z$; (viii) $\frac{3}{2} - x, y, \frac{1}{2} + z$.

In the final stages of refinement, H atoms were placed in calculated positions with C—H = 0.99, 0.98 and 0.95 Å for methylene, methyl and aryl H, respectively, and refined with a riding model, with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H and $1.2U_{\rm eq}({\rm C})$ otherwise.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

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