Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2-Methyl-2-phenylpropyl)triphenylstannane

R. Alan Howie[a]* and James L. Wardell[b]

[a]Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, and [b]Departamento de Química Inorgânica, Instituto de Química, Universidade Federal do Rio de Janeiro, CP 68563, 21945-970 Rio de Janeiro, RJ, Brazil

Correspondence e-mail: r.a.howie@abdn.ac.uk

Received 13 September 2004
Accepted 20 September 2004
Online 30 September 2004

Key indicators

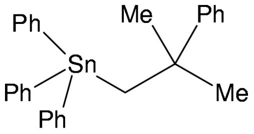
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.067
Data-to-parameter ratio = 13.4

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.

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 $Cg1$, comprising atoms C5–C10, Ph2 with centroid $Cg2$, comprising C11–C16, Ph3 with centroid $Cg3$, comprising C17–C22, and Ph4 with centroid $Cg4$, 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

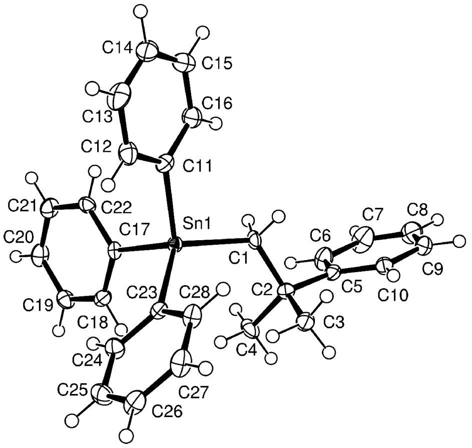


Figure 1
The molecule of (I). Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii.

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$$Cg$4^{vii}. The H$\cdots$$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, $J(^{119,117}Sn–^1H)$ = 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°
$h = -26 \rightarrow 29$
$k = -18 \rightarrow 22$
$l = -10 \rightarrow 14$

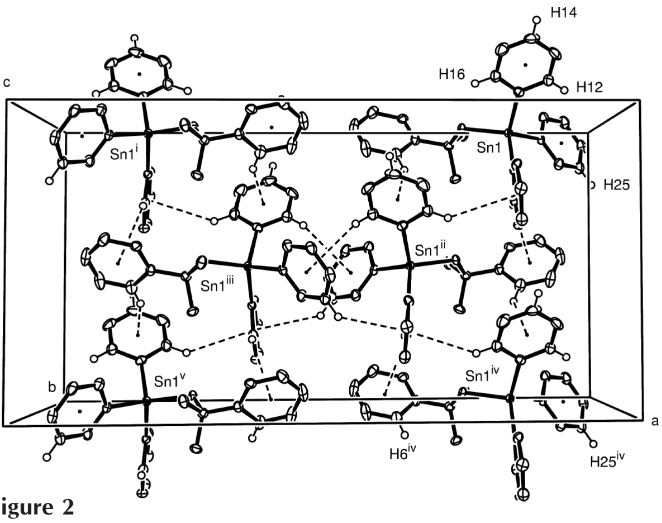


Figure 2
Molecules of (I) in a layer parallel to (010) and centred on *x* = 1. Dashed lines indicate C—H$\cdots\pi$ contacts. Non-H atoms are shown as 50% probability displacement ellipsoids and H atoms as small spheres of arbitrary radii. Selected atoms are labelled. [Symmetry codes: (i) $1 - x, 2 - y, z$; (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$$Cg$2^{ii}	3.10	3.03	12	143	3.90
C12—H12$\cdots$$Cg$4^{vi}	3.21	3.02	20	127	3.86
C14—H14$\cdots$$Cg$4^{vii}	3.19	3.08	15	144	4.00
C16—H16$\cdots$$Cg$3^{viii}	3.18	3.05	16	140	3.95
C18—H18$\cdots$$Cg$1^{ii}	3.24	3.13	14	133	3.94
C25—H25$\cdots$$Cg$3^{vi}	2.98	2.95	8	137	3.74

Notes: (*a*) Cg1–Cg4 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 $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H and 1.2$U_{\rm eq}$(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).

The authors thank CNPq, Brazil, for financial support.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.

Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2004). E**60**, m1536–m1538   [https://doi.org/10.1107/S160053680402330X]

(2-Methyl-2-phenylpropyl)triphenylstannane

R. Alan Howie and James L. Wardell

(2-Methyl-2-phenylpropyl)triphenylstannane

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
F(000) = 1968
D_x = 1.414 Mg m^{-3}
Melting point = 367–368 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4339 reflections
θ = 2.9–27.5°
μ = 1.14 mm^{-1}
T = 120 K
Block, colourless
0.60 × 0.35 × 0.30 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
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°, θ_{min} = 3.0°
$h = -26\rightarrow29$
$k = -18\rightarrow22$
$l = -10\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.067
S = 1.08
3545 reflections
265 parameters
1 restraint
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
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: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00349 (14)
Absolute structure: Flack (1983), 887 Friedel pairs
Absolute structure parameter: 0.04 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

- 2.6828(0.0367) x + 13.0476(0.0202) y + 7.3675(0.0164) z = 18.1598(0.0359)

* -0.0057 (0.0029) C11 * 0.0031 (0.0027) C12 * 0.0041 (0.0027) C13 * -0.0088 (0.0030) C14 * 0.0061 (0.0028) C15 * 0.0012 (0.0028) C16 - 0.1163 (0.0065) Sn1 0.7869 (0.0083) C1 1.3970 (0.0107) C2 2.6003 (0.0112) C3 0.3629 (0.0125) C4 1.7851 (0.0118) C5 0.8100 (0.0129) C6 3.0837 (0.0117) C10

Rms deviation of fitted atoms = 0.0054

22.8025(0.0024) x + 0.4535(0.0221) y + 0.8545(0.0157) z = 20.5373(0.0207)

Angle to previous plane (with approximate e.s.d.) = 87.13 (0.12)

* 0.0007 (0.0022) C17 * 0.0013 (0.0022) C18 * -0.0004 (0.0024) C19 * -0.0024 (0.0025) C20 * 0.0043 (0.0023) C21 * -0.0035 (0.0021) C22 0.0422 (0.0046) Sn1 - 1.9600 (0.0062) C1 - 2.4819 (0.0070) C2 - 1.6823 (0.0084) C3 - 2.3051 (0.0066) C4 - 3.9562 (0.0072) C5 - 4.9060 (0.0062) C6 - 4.4044 (0.0089) C10

Rms deviation of fitted atoms = 0.0025

14.5251(0.0256) x - 10.8057(0.0183) y + 5.1420(0.0153) z = 6.6719(0.0425)

Angle to previous plane (with approximate e.s.d.) = 49.55 (0.11)

* -0.0091 (0.0022) C23 * 0.0061 (0.0024) C24 * -0.0007 (0.0025) C25 * -0.0017 (0.0025) C26 * -0.0014 (0.0025) C27 * 0.0067 (0.0024) C28 0.0144 (0.0051) Sn1 - 1.5915 (0.0075) C1 - 3.0254 (0.0068) C2 - 3.0824 (0.0060) C3 - 3.4702 (0.0064) C4 - 3.8980 (0.0085) C5 - 4.2631 (0.0096) C6 - 4.2916 (0.0092) C10

Rms deviation of fitted atoms = 0.0053

- 2.6828(0.0367) x + 13.0476(0.0202) y + 7.3675(0.0164) z = 18.1598(0.0359)

Angle to previous plane (with approximate e.s.d.) = 73.79 (0.11)

* -0.0057 (0.0029) C11 * 0.0031 (0.0027) C12 * 0.0041 (0.0027) C13 * -0.0088 (0.0030) C14 * 0.0061 (0.0028) C15 * 0.0012 (0.0028) C16

Rms deviation of fitted atoms = 0.0054

20.5468(0.0114) x - 7.4322(0.0177) y - 0.6542(0.0220) z = 10.0988(0.0337)

Angle to previous plane (with approximate e.s.d.) = 61.69 (0.13)

* 0.0000 (0.0000) C11 * 0.0000 (0.0000) C17 * 0.0000 (0.0000) C23 - 0.7616 (0.0017) Sn1 1.2164 (0.0060) C12 - 0.6920 (0.0067) C16 - 0.0626 (0.0064) C18 0.6062 (0.0048) C22 0.7904 (0.0047) C24 - 0.2462 (0.0051) C28

Rms deviation of fitted atoms = 0.0000

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.845344 (7)	0.992790 (9)	0.99869 (6)	0.01462 (8)
C1	0.75596 (12)	1.03149 (18)	1.0202 (3)	0.0181 (8)
H1A	0.7305	0.9881	0.9941	0.022*
H1B	0.7492	1.0377	1.1038	0.022*
C2	0.73376 (14)	1.10661 (18)	0.9619 (3)	0.0183 (7)
C3	0.76558 (12)	1.17785 (16)	1.0106 (4)	0.0236 (7)
H3A	0.7483	1.2258	0.9790	0.035*
H3B	0.8070	1.1753	0.9897	0.035*
H3C	0.7618	1.1782	1.0946	0.035*
C4	0.74644 (16)	1.1031 (2)	0.8323 (3)	0.0272 (8)
H4A	0.7299	1.0549	0.8002	0.041*

H4B	0.7888	1.1037	0.8197	0.041*
H4C	0.7287	1.1486	0.7944	0.041*
C5	0.66819 (13)	1.11003 (17)	0.9846 (4)	0.0185 (8)
C6	0.62981 (15)	1.0626 (2)	0.9223 (4)	0.0283 (8)
H6	0.6446	1.0308	0.8619	0.034*
C7	0.57044 (15)	1.0612 (2)	0.9473 (4)	0.0377 (10)
H7	0.5451	1.0286	0.9036	0.045*
C8	0.54811 (15)	1.1062 (2)	1.0342 (4)	0.0379 (12)
H8	0.5076	1.1046	1.0516	0.046*
C9	0.58504 (16)	1.1536 (2)	1.0957 (4)	0.0295 (9)
H9	0.5698	1.1853	1.1557	0.035*
C10	0.64437 (15)	1.1557 (2)	1.0713 (3)	0.0217 (8)
H10	0.6692	1.1891	1.1149	0.026*
C11	0.86120 (18)	0.9211 (3)	1.1464 (4)	0.0191 (9)
C12	0.91749 (16)	0.9093 (2)	1.1890 (3)	0.0258 (8)
H12	0.9496	0.9357	1.1547	0.031*
C13	0.92684 (17)	0.8593 (2)	1.2811 (3)	0.0329 (9)
H13	0.9653	0.8518	1.3098	0.039*
C14	0.8805 (2)	0.8205 (3)	1.3313 (4)	0.0360 (11)
H14	0.8873	0.7854	1.3933	0.043*
C15	0.82512 (19)	0.8324 (3)	1.2919 (4)	0.0380 (10)
H15	0.7932	0.8066	1.3280	0.046*
C16	0.81499 (15)	0.8818 (2)	1.2002 (3)	0.0271 (8)
H16	0.7762	0.8891	1.1732	0.032*
C17	0.85054 (13)	0.9177 (3)	0.8511 (4)	0.0152 (9)
C18	0.85421 (13)	0.9461 (2)	0.7388 (3)	0.0195 (7)
H18	0.8537	1.0011	0.7258	0.023*
C19	0.85860 (15)	0.8958 (2)	0.6464 (3)	0.0218 (8)
H19	0.8610	0.9161	0.5705	0.026*
C20	0.85941 (16)	0.8161 (3)	0.6648 (4)	0.0254 (9)
H20	0.8622	0.7814	0.6011	0.030*
C21	0.85618 (15)	0.7860 (2)	0.7749 (3)	0.0244 (8)
H21	0.8572	0.7310	0.7871	0.029*
C22	0.85135 (12)	0.8369 (2)	0.8677 (3)	0.0192 (7)
H22	0.8486	0.8163	0.9433	0.023*
C23	0.91309 (12)	1.07891 (15)	0.9837 (3)	0.0160 (7)
C24	0.94898 (13)	1.08020 (19)	0.8880 (3)	0.0223 (7)
H24	0.9432	1.0428	0.8287	0.027*
C25	0.99346 (13)	1.1356 (2)	0.8774 (4)	0.0263 (9)
H25	1.0174	1.1363	0.8106	0.032*
C26	1.00264 (13)	1.1892 (2)	0.9640 (4)	0.0267 (11)
H26	1.0330	1.2269	0.9572	0.032*
C27	0.96772 (16)	1.1881 (2)	1.0605 (3)	0.0268 (8)
H27	0.9740	1.2254	1.1200	0.032*
C28	0.92344 (15)	1.13297 (19)	1.0712 (3)	0.0234 (8)
H28	0.9000	1.1321	1.1386	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01299 (11)	0.01505 (11)	0.01581 (13)	0.00074 (6)	0.00005 (16)	−0.0003 (2)
C1	0.0115 (12)	0.0237 (14)	0.019 (2)	0.0051 (11)	0.0021 (13)	0.0003 (15)
C2	0.0195 (15)	0.0180 (14)	0.0174 (18)	0.0008 (12)	0.0000 (13)	0.0017 (12)
C3	0.0196 (14)	0.0187 (12)	0.033 (2)	−0.0002 (10)	0.0042 (19)	0.001 (2)
C4	0.0250 (17)	0.041 (2)	0.0159 (19)	0.0098 (16)	0.0050 (15)	0.0088 (17)
C5	0.0160 (13)	0.0162 (12)	0.023 (2)	0.0019 (10)	0.0006 (16)	0.0035 (17)
C6	0.0227 (16)	0.0250 (17)	0.037 (2)	0.0012 (15)	−0.0026 (18)	−0.0072 (17)
C7	0.0192 (16)	0.0314 (19)	0.063 (3)	−0.0014 (16)	−0.0090 (18)	−0.006 (2)
C8	0.0164 (16)	0.0363 (19)	0.061 (3)	0.0037 (14)	0.0084 (18)	0.011 (2)
C9	0.0265 (18)	0.0283 (18)	0.034 (2)	0.0122 (15)	0.0087 (17)	0.0077 (17)
C10	0.0241 (16)	0.0235 (17)	0.017 (2)	0.0067 (14)	0.0008 (15)	0.0035 (15)
C11	0.0216 (17)	0.017 (2)	0.019 (2)	0.0023 (18)	−0.0031 (17)	−0.0006 (18)
C12	0.0206 (16)	0.0315 (18)	0.025 (2)	0.0049 (14)	0.0000 (15)	−0.0019 (16)
C13	0.031 (2)	0.039 (2)	0.029 (2)	0.0125 (17)	−0.0136 (18)	−0.0015 (18)
C14	0.050 (3)	0.039 (3)	0.019 (2)	0.018 (2)	0.005 (2)	0.0079 (19)
C15	0.036 (2)	0.041 (2)	0.037 (3)	0.0092 (19)	0.012 (2)	0.017 (2)
C16	0.0196 (16)	0.0318 (18)	0.030 (2)	0.0045 (15)	0.0013 (17)	0.0047 (17)
C17	0.0129 (14)	0.018 (2)	0.015 (2)	0.0020 (13)	−0.0005 (13)	−0.0036 (18)
C18	0.0177 (15)	0.0161 (15)	0.0246 (19)	0.0002 (13)	−0.0018 (14)	0.0019 (15)
C19	0.0222 (17)	0.0281 (18)	0.0150 (18)	0.0007 (14)	−0.0001 (15)	−0.0004 (16)
C20	0.0226 (18)	0.022 (2)	0.031 (3)	−0.0005 (17)	−0.0023 (17)	−0.0120 (18)
C21	0.0266 (17)	0.0149 (16)	0.032 (2)	−0.0033 (14)	0.0009 (16)	−0.0065 (16)
C22	0.0174 (14)	0.0182 (16)	0.022 (2)	−0.0042 (12)	0.0037 (14)	−0.0001 (15)
C23	0.0134 (12)	0.0136 (11)	0.021 (2)	−0.0005 (9)	−0.0024 (14)	−0.0004 (15)
C24	0.0184 (15)	0.0217 (16)	0.027 (2)	−0.0042 (13)	0.0014 (15)	−0.0041 (15)
C25	0.0179 (16)	0.032 (2)	0.029 (2)	−0.0046 (13)	0.0009 (16)	0.0026 (19)
C26	0.0173 (17)	0.0207 (16)	0.042 (3)	−0.0012 (12)	−0.0056 (14)	−0.0027 (16)
C27	0.0223 (18)	0.0259 (18)	0.032 (2)	0.0004 (15)	−0.0065 (18)	−0.0122 (17)
C28	0.0196 (16)	0.0227 (16)	0.028 (2)	0.0022 (13)	−0.0021 (15)	−0.0063 (16)

Geometric parameters (Å, º)

Sn1—C11	2.139 (4)	C12—H12	0.950
Sn1—C23	2.142 (3)	C13—C14	1.379 (6)
Sn1—C17	2.145 (4)	C13—H13	0.950
Sn1—C1	2.163 (3)	C14—C15	1.363 (6)
C1—C2	1.536 (4)	C14—H14	0.950
C1—H1A	0.990	C15—C16	1.378 (5)
C1—H1B	0.990	C15—H15	0.950
C2—C5	1.524 (4)	C16—H16	0.950
C2—C3	1.526 (4)	C17—C22	1.392 (6)
C2—C4	1.536 (5)	C17—C18	1.397 (6)
C3—H3A	0.980	C18—C19	1.379 (5)
C3—H3B	0.980	C18—H18	0.950
C3—H3C	0.980	C19—C20	1.377 (6)

C4—H4A	0.980	C19—H19	0.950
C4—H4B	0.980	C20—C21	1.382 (6)
C4—H4C	0.980	C20—H20	0.950
C5—C10	1.386 (5)	C21—C22	1.389 (5)
C5—C6	1.397 (5)	C21—H21	0.950
C6—C7	1.389 (5)	C22—H22	0.950
C6—H6	0.950	C23—C24	1.383 (5)
C7—C8	1.368 (5)	C23—C28	1.393 (5)
C7—H7	0.950	C24—C25	1.394 (4)
C8—C9	1.371 (5)	C24—H24	0.950
C8—H8	0.950	C25—C26	1.377 (6)
C9—C10	1.387 (5)	C25—H25	0.950
C9—H9	0.950	C26—C27	1.378 (6)
C10—H10	0.950	C26—H26	0.950
C11—C12	1.394 (5)	C27—C28	1.388 (5)
C11—C16	1.400 (5)	C27—H27	0.950
C12—C13	1.386 (5)	C28—H28	0.950

C11—Sn1—C23	109.53 (15)	C13—C12—C11	120.4 (4)
C11—Sn1—C17	106.97 (11)	C13—C12—H12	119.8
C23—Sn1—C17	107.73 (15)	C11—C12—H12	119.8
C11—Sn1—C1	103.98 (15)	C14—C13—C12	120.3 (4)
C23—Sn1—C1	118.93 (11)	C14—C13—H13	119.8
C17—Sn1—C1	109.10 (13)	C12—C13—H13	119.8
C2—C1—Sn1	121.1 (2)	C15—C14—C13	120.0 (4)
C2—C1—H1A	107.1	C15—C14—H14	120.0
Sn1—C1—H1A	107.1	C13—C14—H14	120.0
C2—C1—H1B	107.1	C14—C15—C16	120.5 (4)
Sn1—C1—H1B	107.1	C14—C15—H15	119.7
H1A—C1—H1B	106.8	C16—C15—H15	119.7
C5—C2—C3	112.0 (3)	C15—C16—C11	120.8 (4)
C5—C2—C1	106.3 (3)	C15—C16—H16	119.6
C3—C2—C1	110.0 (3)	C11—C16—H16	119.6
C5—C2—C4	110.9 (3)	C22—C17—C18	118.2 (4)
C3—C2—C4	107.8 (3)	C22—C17—Sn1	118.8 (3)
C1—C2—C4	109.8 (3)	C18—C17—Sn1	123.0 (3)
C2—C3—H3A	109.5	C19—C18—C17	121.2 (3)
C2—C3—H3B	109.5	C19—C18—H18	119.4
H3A—C3—H3B	109.5	C17—C18—H18	119.4
C2—C3—H3C	109.5	C20—C19—C18	119.6 (4)
H3A—C3—H3C	109.5	C20—C19—H19	120.2
H3B—C3—H3C	109.5	C18—C19—H19	120.2
C2—C4—H4A	109.5	C19—C20—C21	120.7 (4)
C2—C4—H4B	109.5	C19—C20—H20	119.7
H4A—C4—H4B	109.5	C21—C20—H20	119.7
C2—C4—H4C	109.5	C20—C21—C22	119.5 (3)
H4A—C4—H4C	109.5	C20—C21—H21	120.2
H4B—C4—H4C	109.5	C22—C21—H21	120.2

C10—C5—C6	117.2 (3)	C21—C22—C17	120.8 (4)
C10—C5—C2	122.3 (3)	C21—C22—H22	119.6
C6—C5—C2	120.4 (3)	C17—C22—H22	119.6
C7—C6—C5	121.1 (4)	C24—C23—C28	118.4 (3)
C7—C6—H6	119.5	C24—C23—Sn1	120.4 (2)
C5—C6—H6	119.5	C28—C23—Sn1	121.2 (2)
C8—C7—C6	120.6 (4)	C23—C24—C25	121.1 (3)
C8—C7—H7	119.7	C23—C24—H24	119.5
C6—C7—H7	119.7	C25—C24—H24	119.5
C7—C8—C9	119.1 (3)	C26—C25—C24	119.8 (4)
C7—C8—H8	120.4	C26—C25—H25	120.1
C9—C8—H8	120.4	C24—C25—H25	120.1
C8—C9—C10	120.8 (4)	C25—C26—C27	119.9 (3)
C8—C9—H9	119.6	C25—C26—H26	120.0
C10—C9—H9	119.6	C27—C26—H26	120.0
C5—C10—C9	121.2 (3)	C26—C27—C28	120.3 (3)
C5—C10—H10	119.4	C26—C27—H27	119.8
C9—C10—H10	119.4	C28—C27—H27	119.8
C12—C11—C16	117.9 (4)	C27—C28—C23	120.5 (3)
C12—C11—Sn1	121.6 (3)	C27—C28—H28	119.8
C16—C11—Sn1	120.4 (3)	C23—C28—H28	119.8

C12—C11—Sn1—C1	−155.0 (3)	Sn1—C1—C2—C3	−64.9 (4)
C16—C11—Sn1—C1	27.8 (4)	Sn1—C1—C2—C4	53.6 (3)
C18—C17—Sn1—C1	81.4 (3)	Sn1—C1—C2—C5	173.7 (2)
C22—C17—Sn1—C1	−99.8 (3)	C1—C2—C5—C6	−76.8 (4)
C24—C23—Sn1—C1	−122.4 (3)	C1—C2—C5—C10	99.0 (4)
C28—C23—Sn1—C1	59.8 (3)	C3—C2—C5—C6	163.0 (3)
C11—Sn1—C1—C2	156.5 (3)	C3—C2—C5—C10	−21.2 (5)
C17—Sn1—C1—C2	−89.6 (3)	C4—C2—C5—C6	42.5 (5)
C23—Sn1—C1—C2	34.4 (3)	C4—C2—C5—C10	−141.6 (3)