

catena-Poly[[triphenyltin(IV)]- μ -2-(cyclohexylaminocarbonyl)benzoato- κ^2 O¹:O²]

Imtiaz-ud-Din,^a Raziq-ul-Rasool,^a Moazzam H. Bhatti^a and Seik Weng Ng^{b*}

^aDepartment of Chemistry, Allama Iqbal Open University, H/8 Islamabad, Pakistan, and ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

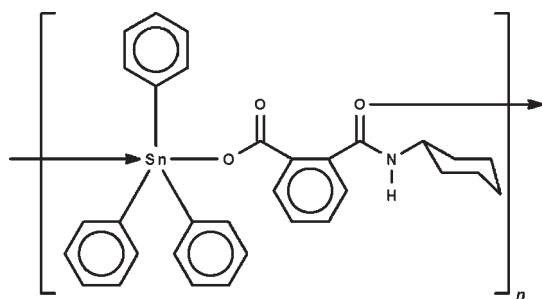
Received 7 July 2010; accepted 7 July 2010

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.019; wR factor = 0.049; data-to-parameter ratio = 18.2.

In the title polymeric complex, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{14}\text{H}_{16}\text{NO}_3)]_n$, adjacent triphenyltin cations are bridged by the *N*-cyclohexylphthalamate anion through the carboxylate and carbonyl O atoms, forming a helical chain running along the *b* axis. The amide N atom is a hydrogen-bond donor to the uncoordinated carboxylate O atom. The geometry at the five-coordinate Sn atom is *trans*- C_3SnO_2 trigonal-bipyramidal.

Related literature

For a review on organotin carboxylates, see: Tiekink (1991, 1994). Triphenyltin arylcarboxylates generally exist as monomeric molecules; see: Ng *et al.* (1986). For the synthesis of *N*-cyclohexylphthalamic acid, see: Dolzhenko *et al.* (2003).



Experimental

Crystal data

$[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{14}\text{H}_{16}\text{NO}_3)]$
 $M_r = 596.27$
Monoclinic, $P2_1/n$
 $a = 9.8574$ (5) Å
 $b = 16.0734$ (8) Å
 $c = 17.1669$ (8) Å
 $\beta = 99.447$ (1)°

$V = 2683.1$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.99$ mm⁻¹
 $T = 100$ K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.694$, $T_{\max} = 0.827$

25326 measured reflections
6165 independent reflections
5710 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.049$
 $S = 1.02$
6165 reflections
338 parameters
1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.50$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Sn1—C1	2.130 (1)	Sn1—O1	2.149 (1)
Sn1—C7	2.129 (2)	Sn1—O3 ⁱ	2.392 (1)
Sn1—C13	2.119 (1)		
O1—Sn1—O3 ⁱ	174.06 (4)		

Symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O2	0.86 (1)	1.85 (1)	2.666 (2)	158 (2)

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Allama Iqbal Open University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2796).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dolzhenko, A. V., Syropyatov, B. Ya., Koz'minykh, V. O., Kolotova, N. V., Zakhmatov, A. V. & Borodin, A. Yu. (2003). *Pharm. Chem. J.* **37**, 407–408.
Ng, S. W., Chen, W. & Kumar Das, V. G. (1986). *J. Organomet. Chem.* **345**, 59–64.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Tiekink, E. R. T. (1991). *Appl. Organomet. Chem.* **5**, 1–23.
Tiekink, E. R. T. (1994). *Trends Organomet. Chem.* **1**, 71–116.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2010). E66, m931 [doi:10.1107/S1600536810026978]

***catena*-Poly[[triphenyltin(IV)]- μ -2-(cyclohexylaminocarbonyl)benzoato- κ^2 O¹:O²]**

Imtiaz-ud-Din, Raqiyat-ul-Rasool, M. H. Bhatti and S. W. Ng

Comment

Triphenyltin aryl-carboxylates commonly exist as four-coordinate tetrahedral compounds unlike the alkyl-carboxylates, which adopt carboxylate-bridged polymeric chains structures (Ng *et al.*, 1986). Occasionally, the aryl-carboxylate anion bears a potential donor unit such as, in the present case, an amido group; such a donor group can interact with adjacent molecules to generate polymeric chain motifs (Tiekink, 1991; 1994). In the present *N*-cyclohexylphthalimic acid derivative (Scheme I), the amido oxygen atom engages in bonding to generate a chain motif (Fig. 1). The tin atom is displaced out of the C₃Sn girdle in the direction of the covalently-bonded oxygen atom by 0.200 (1) Å; the Sn–O_{covalent} bond is significantly shorter than the Sn–O_{dative} bond.

Experimental

N-Cyclohexylphthalamic acid was synthesized from the reaction of phthalic anhydride and cyclohexylamine in ethyl acetate by using a reported procedure (Dolzhenko *et al.*, 2003).

Triphenyltin hydroxide (1 mmol, 0.37 g) and *N*-cyclohexylphthalamic acid (1 mmol, 0.25 g) were heated in toluene (50 ml) for 6 h in a Dean-Stark water-separator. The solvent was then removed and the solid material recrystallized from a chloroform and *n*-hexane (3:1) mixture to furnish crystals.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$.

The amido H-atom was located in a difference Fourier map, and was refined with N—H 0.86 ± 0.01 Å; its temperature factor was freely refined.

Figures

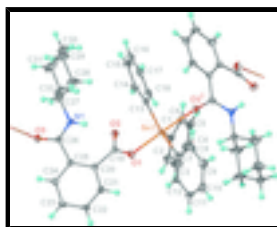


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a portion of polymeric Sn(C₆H₅)₃(C₁₄H₁₆NO₃) at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

catena-Poly[[triphenyltin(IV)]- μ -2-(cyclohexylaminocarbonyl)benzoato- $\kappa^2 O^1:O^2$]

Crystal data

[Sn(C ₆ H ₅) ₃ (C ₁₄ H ₁₆ NO ₃)]	$F(000) = 1216$
$M_r = 596.27$	$D_x = 1.476 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2yn	Cell parameters from 9925 reflections
$a = 9.8574 (5) \text{ \AA}$	$\theta = 2.4\text{--}28.3^\circ$
$b = 16.0734 (8) \text{ \AA}$	$\mu = 0.99 \text{ mm}^{-1}$
$c = 17.1669 (8) \text{ \AA}$	$T = 100 \text{ K}$
$\beta = 99.447 (1)^\circ$	Block, colorless
$V = 2683.1 (2) \text{ \AA}^3$	$0.40 \times 0.30 \times 0.20 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX diffractometer	6165 independent reflections
Radiation source: fine-focus sealed tube graphite	5710 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.023$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.8^\circ$
$T_{\text{min}} = 0.694$, $T_{\text{max}} = 0.827$	$h = -12 \rightarrow 11$
25326 measured reflections	$k = -20 \rightarrow 20$
	$l = -22 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.019$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 1.7091P]$
6165 reflections	where $P = (F_o^2 + 2F_c^2)/3$
338 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
1 restraint	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.914994 (9)	0.372319 (5)	0.750433 (5)	0.01199 (4)

O1	0.88805 (10)	0.26134 (6)	0.67977 (6)	0.0167 (2)
O2	0.66233 (11)	0.26088 (6)	0.67972 (6)	0.0181 (2)
O3	0.53077 (10)	-0.00855 (6)	0.66684 (6)	0.0160 (2)
N1	0.51088 (14)	0.12682 (7)	0.69698 (8)	0.0177 (3)
H1	0.5391 (19)	0.1765 (7)	0.6891 (11)	0.022 (5)*
C1	0.78221 (14)	0.45043 (8)	0.67164 (8)	0.0150 (3)
C2	0.78027 (18)	0.44190 (10)	0.59071 (9)	0.0242 (3)
H2	0.8315	0.3985	0.5717	0.029*
C3	0.70416 (19)	0.49620 (11)	0.53752 (10)	0.0293 (4)
H3	0.7034	0.4895	0.4825	0.035*
C4	0.62957 (17)	0.55996 (10)	0.56442 (10)	0.0257 (3)
H4	0.5788	0.5975	0.5280	0.031*
C5	0.62943 (15)	0.56869 (9)	0.64469 (10)	0.0209 (3)
H5	0.5781	0.6122	0.6635	0.025*
C6	0.70430 (14)	0.51388 (9)	0.69779 (9)	0.0170 (3)
H6	0.7024	0.5197	0.7527	0.020*
C7	1.12405 (15)	0.37813 (8)	0.73368 (9)	0.0143 (3)
C8	1.22988 (15)	0.39979 (9)	0.79465 (9)	0.0175 (3)
H8	1.2096	0.4093	0.8461	0.021*
C9	1.36463 (16)	0.40761 (10)	0.78118 (10)	0.0230 (3)
H9	1.4356	0.4216	0.8236	0.028*
C10	1.39583 (16)	0.39509 (9)	0.70631 (10)	0.0232 (3)
H10	1.4880	0.4002	0.6973	0.028*
C11	1.29187 (18)	0.37515 (9)	0.64477 (10)	0.0230 (3)
H11	1.3124	0.3677	0.5931	0.028*
C12	1.15697 (16)	0.36592 (9)	0.65838 (9)	0.0188 (3)
H12	1.0866	0.3512	0.6159	0.023*
C13	0.85936 (15)	0.32474 (8)	0.85593 (8)	0.0147 (3)
C14	0.72102 (16)	0.32227 (9)	0.86407 (9)	0.0180 (3)
H14	0.6523	0.3338	0.8198	0.022*
C15	0.68262 (17)	0.30300 (10)	0.93644 (9)	0.0226 (3)
H15	0.5880	0.3018	0.9413	0.027*
C16	0.78136 (19)	0.28563 (10)	1.00104 (9)	0.0245 (3)
H16	0.7549	0.2737	1.0506	0.029*
C17	0.91974 (18)	0.28560 (10)	0.99353 (9)	0.0244 (3)
H17	0.9878	0.2718	1.0375	0.029*
C18	0.95815 (16)	0.30584 (9)	0.92144 (9)	0.0198 (3)
H18	1.0528	0.3068	0.9168	0.024*
C19	0.76680 (15)	0.22960 (8)	0.66099 (8)	0.0144 (3)
C20	0.76215 (15)	0.15244 (9)	0.60958 (8)	0.0140 (3)
C21	0.86142 (16)	0.15062 (10)	0.55998 (9)	0.0195 (3)
H21	0.9268	0.1944	0.5633	0.023*
C22	0.86751 (17)	0.08691 (10)	0.50612 (9)	0.0224 (3)
H22	0.9354	0.0877	0.4727	0.027*
C23	0.77383 (17)	0.02216 (9)	0.50143 (9)	0.0200 (3)
H23	0.7757	-0.0212	0.4640	0.024*
C24	0.67742 (15)	0.02117 (9)	0.55164 (8)	0.0161 (3)
H24	0.6152	-0.0243	0.5490	0.019*
C25	0.66847 (14)	0.08489 (8)	0.60619 (8)	0.0132 (3)

supplementary materials

C26	0.56431 (14)	0.06626 (8)	0.66012 (8)	0.0134 (3)
C27	0.41889 (15)	0.11215 (9)	0.75476 (9)	0.0181 (3)
H27	0.4034	0.0509	0.7585	0.022*
C28	0.48651 (19)	0.14361 (12)	0.83514 (10)	0.0293 (4)
H28A	0.5067	0.2037	0.8317	0.035*
H28B	0.5746	0.1140	0.8516	0.035*
C29	0.3924 (2)	0.12963 (12)	0.89671 (11)	0.0342 (4)
H29A	0.3791	0.0692	0.9036	0.041*
H29B	0.4365	0.1528	0.9481	0.041*
C30	0.2540 (2)	0.17094 (11)	0.87143 (12)	0.0337 (4)
H30A	0.1931	0.1578	0.9103	0.040*
H30B	0.2664	0.2320	0.8708	0.040*
C31	0.18684 (19)	0.14199 (13)	0.79050 (13)	0.0357 (4)
H31A	0.1005	0.1734	0.7742	0.043*
H31B	0.1630	0.0823	0.7930	0.043*
C32	0.28089 (18)	0.15421 (12)	0.72883 (11)	0.0298 (4)
H32B	0.2364	0.1305	0.6777	0.036*
H32C	0.2952	0.2144	0.7212	0.036*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01138 (5)	0.01205 (5)	0.01288 (5)	0.00013 (3)	0.00303 (4)	0.00005 (3)
O1	0.0158 (5)	0.0156 (5)	0.0186 (5)	-0.0014 (4)	0.0025 (4)	-0.0032 (4)
O2	0.0180 (5)	0.0149 (5)	0.0229 (5)	-0.0007 (4)	0.0081 (4)	-0.0011 (4)
O3	0.0181 (5)	0.0133 (4)	0.0169 (5)	-0.0009 (4)	0.0042 (4)	0.0016 (4)
N1	0.0202 (6)	0.0132 (6)	0.0222 (6)	-0.0013 (5)	0.0109 (5)	0.0013 (5)
C1	0.0143 (7)	0.0140 (6)	0.0167 (7)	-0.0009 (5)	0.0019 (5)	0.0015 (5)
C2	0.0300 (9)	0.0236 (8)	0.0195 (8)	0.0096 (6)	0.0057 (6)	0.0005 (6)
C3	0.0373 (10)	0.0334 (9)	0.0171 (7)	0.0116 (7)	0.0040 (7)	0.0050 (7)
C4	0.0249 (8)	0.0257 (8)	0.0262 (8)	0.0068 (6)	0.0035 (6)	0.0092 (6)
C5	0.0152 (7)	0.0186 (7)	0.0296 (8)	0.0033 (5)	0.0056 (6)	0.0011 (6)
C6	0.0129 (6)	0.0201 (7)	0.0185 (7)	-0.0011 (5)	0.0038 (5)	-0.0020 (5)
C7	0.0144 (6)	0.0116 (6)	0.0175 (7)	0.0009 (5)	0.0042 (5)	0.0000 (5)
C8	0.0175 (7)	0.0176 (7)	0.0178 (7)	0.0014 (5)	0.0043 (6)	-0.0015 (5)
C9	0.0158 (7)	0.0223 (7)	0.0300 (8)	0.0001 (6)	0.0012 (6)	-0.0013 (6)
C10	0.0166 (7)	0.0176 (7)	0.0379 (9)	-0.0013 (6)	0.0124 (7)	0.0003 (6)
C11	0.0278 (8)	0.0197 (7)	0.0253 (8)	-0.0019 (6)	0.0158 (7)	-0.0014 (6)
C12	0.0203 (7)	0.0189 (7)	0.0180 (7)	-0.0022 (5)	0.0056 (6)	-0.0029 (5)
C13	0.0188 (7)	0.0112 (6)	0.0147 (6)	0.0001 (5)	0.0045 (5)	-0.0009 (5)
C14	0.0189 (7)	0.0193 (7)	0.0162 (7)	0.0014 (5)	0.0041 (5)	0.0000 (5)
C15	0.0255 (8)	0.0217 (7)	0.0235 (8)	-0.0008 (6)	0.0126 (6)	-0.0014 (6)
C16	0.0410 (10)	0.0182 (7)	0.0157 (7)	-0.0039 (6)	0.0089 (7)	0.0003 (6)
C17	0.0353 (9)	0.0184 (7)	0.0168 (7)	-0.0028 (6)	-0.0040 (6)	0.0025 (6)
C18	0.0200 (7)	0.0161 (7)	0.0222 (7)	-0.0018 (5)	0.0005 (6)	0.0007 (6)
C19	0.0185 (7)	0.0131 (6)	0.0122 (6)	-0.0005 (5)	0.0039 (5)	0.0022 (5)
C20	0.0155 (7)	0.0136 (6)	0.0130 (6)	0.0003 (5)	0.0023 (5)	0.0006 (5)
C21	0.0217 (8)	0.0189 (7)	0.0195 (7)	-0.0046 (6)	0.0078 (6)	-0.0020 (6)

C22	0.0274 (8)	0.0230 (7)	0.0200 (7)	-0.0026 (6)	0.0133 (6)	-0.0022 (6)
C23	0.0290 (8)	0.0168 (7)	0.0156 (7)	-0.0002 (6)	0.0074 (6)	-0.0027 (5)
C24	0.0194 (7)	0.0143 (6)	0.0142 (6)	-0.0014 (5)	0.0018 (5)	0.0006 (5)
C25	0.0132 (6)	0.0142 (6)	0.0120 (6)	0.0010 (5)	0.0019 (5)	0.0017 (5)
C26	0.0125 (6)	0.0151 (6)	0.0121 (6)	0.0002 (5)	0.0005 (5)	0.0020 (5)
C27	0.0206 (7)	0.0134 (6)	0.0234 (8)	0.0004 (5)	0.0126 (6)	0.0019 (5)
C28	0.0249 (9)	0.0423 (10)	0.0231 (8)	-0.0018 (7)	0.0113 (7)	-0.0007 (7)
C29	0.0366 (10)	0.0444 (11)	0.0260 (9)	-0.0012 (8)	0.0181 (8)	0.0011 (7)
C30	0.0437 (11)	0.0218 (8)	0.0447 (11)	0.0067 (7)	0.0340 (9)	0.0064 (7)
C31	0.0211 (9)	0.0427 (10)	0.0480 (12)	0.0074 (7)	0.0194 (8)	0.0164 (9)
C32	0.0207 (8)	0.0401 (9)	0.0310 (9)	0.0039 (7)	0.0118 (7)	0.0107 (8)

Geometric parameters (Å, °)

Sn1—C1	2.130 (1)	C14—H14	0.9500
Sn1—C7	2.129 (2)	C15—C16	1.379 (2)
Sn1—C13	2.119 (1)	C15—H15	0.9500
Sn1—O1	2.149 (1)	C16—C17	1.391 (3)
Sn1—O3 ⁱ	2.392 (1)	C16—H16	0.9500
O1—C19	1.2908 (17)	C17—C18	1.391 (2)
O2—C19	1.2350 (18)	C17—H17	0.9500
O3—C26	1.2574 (17)	C18—H18	0.9500
O3—Sn1 ⁱⁱ	2.3917 (10)	C19—C20	1.5186 (19)
N1—C26	1.3171 (18)	C20—C21	1.399 (2)
N1—C27	1.4687 (18)	C20—C25	1.4204 (19)
N1—H1	0.864 (9)	C21—C22	1.388 (2)
C1—C6	1.395 (2)	C21—H21	0.9500
C1—C2	1.393 (2)	C22—C23	1.385 (2)
C2—C3	1.391 (2)	C22—H22	0.9500
C2—H2	0.9500	C23—C24	1.384 (2)
C3—C4	1.384 (2)	C23—H23	0.9500
C3—H3	0.9500	C24—C25	1.4004 (19)
C4—C5	1.385 (2)	C24—H24	0.9500
C4—H4	0.9500	C25—C26	1.5208 (19)
C5—C6	1.390 (2)	C27—C32	1.519 (2)
C5—H5	0.9500	C27—C28	1.517 (2)
C6—H6	0.9500	C27—H27	1.0000
C7—C8	1.395 (2)	C28—C29	1.533 (2)
C7—C12	1.397 (2)	C28—H28A	0.9900
C8—C9	1.391 (2)	C28—H28B	0.9900
C8—H8	0.9500	C29—C30	1.515 (3)
C9—C10	1.385 (2)	C29—H29A	0.9900
C9—H9	0.9500	C29—H29B	0.9900
C10—C11	1.383 (2)	C30—C31	1.511 (3)
C10—H10	0.9500	C30—H30A	0.9900
C11—C12	1.395 (2)	C30—H30B	0.9900
C11—H11	0.9500	C31—C32	1.530 (2)
C12—H12	0.9500	C31—H31A	0.9900
C13—C14	1.394 (2)	C31—H31B	0.9900

supplementary materials

C13—C18	1.395 (2)	C32—H32B	0.9900
C14—C15	1.392 (2)	C32—H32C	0.9900
C13—Sn1—C7	121.55 (6)	C16—C17—H17	120.1
C13—Sn1—C1	122.49 (5)	C17—C18—C13	120.82 (15)
C7—Sn1—C1	113.32 (5)	C17—C18—H18	119.6
C13—Sn1—O1	99.06 (5)	C13—C18—H18	119.6
C7—Sn1—O1	89.59 (5)	O2—C19—O1	123.47 (13)
C1—Sn1—O1	97.16 (5)	O2—C19—C20	122.47 (13)
C13—Sn1—O3 ⁱ	81.11 (4)	O1—C19—C20	113.98 (12)
C7—Sn1—O3 ⁱ	85.30 (4)	C21—C20—C25	118.31 (13)
C1—Sn1—O3 ⁱ	87.67 (4)	C21—C20—C19	114.42 (12)
O1—Sn1—O3 ⁱ	174.06 (4)	C25—C20—C19	127.27 (12)
C19—O1—Sn1	119.52 (9)	C22—C21—C20	122.14 (14)
C26—O3—Sn1 ⁱⁱ	141.59 (9)	C22—C21—H21	118.9
C26—N1—C27	123.08 (12)	C20—C21—H21	118.9
C26—N1—H1	116.4 (13)	C21—C22—C23	119.47 (14)
C27—N1—H1	120.3 (13)	C21—C22—H22	120.3
C6—C1—C2	118.35 (13)	C23—C22—H22	120.3
C6—C1—Sn1	122.69 (11)	C24—C23—C22	119.46 (13)
C2—C1—Sn1	118.80 (11)	C24—C23—H23	120.3
C3—C2—C1	120.72 (14)	C22—C23—H23	120.3
C3—C2—H2	119.6	C23—C24—C25	122.23 (13)
C1—C2—H2	119.6	C23—C24—H24	118.9
C4—C3—C2	120.30 (15)	C25—C24—H24	118.9
C4—C3—H3	119.8	C24—C25—C20	118.33 (13)
C2—C3—H3	119.8	C24—C25—C26	112.71 (12)
C3—C4—C5	119.62 (15)	C20—C25—C26	128.68 (12)
C3—C4—H4	120.2	O3—C26—N1	122.06 (13)
C5—C4—H4	120.2	O3—C26—C25	117.27 (12)
C4—C5—C6	120.08 (14)	N1—C26—C25	120.67 (12)
C4—C5—H5	120.0	N1—C27—C32	110.68 (12)
C6—C5—H5	120.0	N1—C27—C28	109.45 (13)
C1—C6—C5	120.91 (14)	C32—C27—C28	110.90 (14)
C1—C6—H6	119.5	N1—C27—H27	108.6
C5—C6—H6	119.5	C32—C27—H27	108.6
C8—C7—C12	118.07 (14)	C28—C27—H27	108.6
C8—C7—Sn1	122.05 (11)	C27—C28—C29	110.67 (15)
C12—C7—Sn1	119.72 (11)	C27—C28—H28A	109.5
C9—C8—C7	120.98 (14)	C29—C28—H28A	109.5
C9—C8—H8	119.5	C27—C28—H28B	109.5
C7—C8—H8	119.5	C29—C28—H28B	109.5
C10—C9—C8	120.32 (15)	H28A—C28—H28B	108.1
C10—C9—H9	119.8	C30—C29—C28	110.89 (15)
C8—C9—H9	119.8	C30—C29—H29A	109.5
C9—C10—C11	119.54 (14)	C28—C29—H29A	109.5
C9—C10—H10	120.2	C30—C29—H29B	109.5
C11—C10—H10	120.2	C28—C29—H29B	109.5
C10—C11—C12	120.25 (15)	H29A—C29—H29B	108.0

C10—C11—H11	119.9	C31—C30—C29	111.49 (15)
C12—C11—H11	119.9	C31—C30—H30A	109.3
C11—C12—C7	120.82 (15)	C29—C30—H30A	109.3
C11—C12—H12	119.6	C31—C30—H30B	109.3
C7—C12—H12	119.6	C29—C30—H30B	109.3
C14—C13—C18	118.56 (13)	H30A—C30—H30B	108.0
C14—C13—Sn1	119.37 (10)	C30—C31—C32	111.89 (16)
C18—C13—Sn1	121.55 (11)	C30—C31—H31A	109.2
C15—C14—C13	120.64 (14)	C32—C31—H31A	109.2
C15—C14—H14	119.7	C30—C31—H31B	109.2
C13—C14—H14	119.7	C32—C31—H31B	109.2
C16—C15—C14	120.24 (15)	H31A—C31—H31B	107.9
C16—C15—H15	119.9	C27—C32—C31	110.81 (14)
C14—C15—H15	119.9	C27—C32—H32B	109.5
C15—C16—C17	119.93 (14)	C31—C32—H32B	109.5
C15—C16—H16	120.0	C27—C32—H32C	109.5
C17—C16—H16	120.0	C31—C32—H32C	109.5
C18—C17—C16	119.78 (15)	H32B—C32—H32C	108.1
C18—C17—H17	120.1		
C13—Sn1—O1—C19	64.82 (11)	C18—C13—C14—C15	1.3 (2)
C7—Sn1—O1—C19	-173.26 (10)	Sn1—C13—C14—C15	-170.53 (11)
C1—Sn1—O1—C19	-59.80 (10)	C13—C14—C15—C16	-0.4 (2)
C13—Sn1—C1—C6	41.13 (14)	C14—C15—C16—C17	-1.4 (2)
C7—Sn1—C1—C6	-120.66 (12)	C15—C16—C17—C18	2.1 (2)
O1—Sn1—C1—C6	146.69 (11)	C16—C17—C18—C13	-1.2 (2)
O3 ⁱ —Sn1—C1—C6	-36.79 (12)	C14—C13—C18—C17	-0.5 (2)
C13—Sn1—C1—C2	-143.59 (12)	Sn1—C13—C18—C17	171.13 (11)
C7—Sn1—C1—C2	54.62 (13)	Sn1—O1—C19—O2	2.02 (18)
O1—Sn1—C1—C2	-38.03 (13)	Sn1—O1—C19—C20	178.78 (8)
O3 ⁱ —Sn1—C1—C2	138.49 (12)	O2—C19—C20—C21	146.62 (14)
C6—C1—C2—C3	1.0 (2)	O1—C19—C20—C21	-30.18 (18)
Sn1—C1—C2—C3	-174.49 (14)	O2—C19—C20—C25	-32.3 (2)
C1—C2—C3—C4	0.3 (3)	O1—C19—C20—C25	150.90 (14)
C2—C3—C4—C5	-1.0 (3)	C25—C20—C21—C22	2.4 (2)
C3—C4—C5—C6	0.3 (3)	C19—C20—C21—C22	-176.59 (14)
C2—C1—C6—C5	-1.7 (2)	C20—C21—C22—C23	-0.8 (2)
Sn1—C1—C6—C5	173.61 (11)	C21—C22—C23—C24	-1.3 (2)
C4—C5—C6—C1	1.1 (2)	C22—C23—C24—C25	1.7 (2)
C13—Sn1—C7—C8	-38.88 (13)	C23—C24—C25—C20	-0.1 (2)
C1—Sn1—C7—C8	123.10 (11)	C23—C24—C25—C26	-174.48 (13)
O1—Sn1—C7—C8	-139.28 (11)	C21—C20—C25—C24	-2.0 (2)
O3 ⁱ —Sn1—C7—C8	37.67 (11)	C19—C20—C25—C24	176.91 (13)
C13—Sn1—C7—C12	145.85 (10)	C21—C20—C25—C26	171.43 (14)
C1—Sn1—C7—C12	-52.17 (12)	C19—C20—C25—C26	-9.7 (2)
O1—Sn1—C7—C12	45.45 (11)	Sn1 ⁱⁱ —O3—C26—N1	-85.49 (19)
O3 ⁱ —Sn1—C7—C12	-137.60 (11)	Sn1 ⁱⁱ —O3—C26—C25	95.48 (16)
C12—C7—C8—C9	-1.1 (2)	C27—N1—C26—O3	6.3 (2)
Sn1—C7—C8—C9	-176.43 (11)	C27—N1—C26—C25	-174.74 (13)

supplementary materials

C7—C8—C9—C10	0.9 (2)	C24—C25—C26—O3	20.40 (18)
C8—C9—C10—C11	0.3 (2)	C20—C25—C26—O3	-153.31 (14)
C9—C10—C11—C12	-1.4 (2)	C24—C25—C26—N1	-158.65 (13)
C10—C11—C12—C7	1.2 (2)	C20—C25—C26—N1	27.6 (2)
C8—C7—C12—C11	0.0 (2)	C26—N1—C27—C32	-121.11 (16)
Sn1—C7—C12—C11	175.48 (11)	C26—N1—C27—C28	116.37 (16)
C7—Sn1—C13—C14	179.98 (10)	N1—C27—C28—C29	179.65 (14)
C1—Sn1—C13—C14	19.66 (13)	C32—C27—C28—C29	57.26 (19)
O1—Sn1—C13—C14	-84.89 (11)	C27—C28—C29—C30	-56.6 (2)
O3 ⁱ —Sn1—C13—C14	101.13 (11)	C28—C29—C30—C31	55.2 (2)
C7—Sn1—C13—C18	8.41 (14)	C29—C30—C31—C32	-54.5 (2)
C1—Sn1—C13—C18	-151.91 (11)	N1—C27—C32—C31	-177.73 (15)
O1—Sn1—C13—C18	103.54 (11)	C28—C27—C32—C31	-56.1 (2)
O3 ⁱ —Sn1—C13—C18	-70.44 (11)	C30—C31—C32—C27	54.7 (2)

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O2	0.86 (1)	1.85 (1)	2.666 (2)	158 (2)

Fig. 1

