Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Methanol-κO)(2-methyl-3-nitrobenzoato-κO)triphenyltin(IV)

Foo Win Yip,[a] Siang Guan Teoh,[b] Bohari M. Yamin[c] and Seik Weng Ng[d]*

[a]Department of Chemical Science, Faculty of Science, Universiti Tunku Abdul Rahman, 31900 Kampar, Malaysia, [b]School of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia, [c]School of Chemical Sciences and Food Technology, Faculty of Science and Technology, Universiti Kebangbaan Malaysia, 43600 Bangi, Malaysia, and [d]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

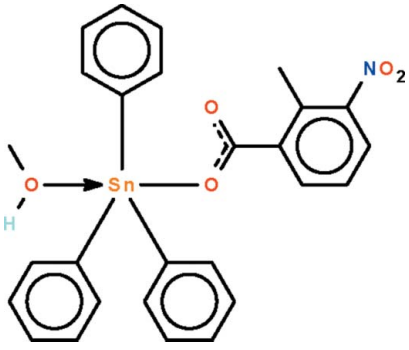
Received 19 August 2010; accepted 20 August 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 18.3.

The five-coordinate Sn atom in the title compound, $[Sn(C_6H_5)_3(C_8H_6NO_4)(CH_3OH)]$, exists in a *trans*-$C_3SnO_2$ trigonal-bipyramidal coordination polyhedron of which the O atoms of the methanol molecule and carboxylate group occupy the apical sites. In the crystal, adjacent molecules are linked by intermolecular O—H···O interactions, generating a helical hydrogen-bonded chain running along the *b* axis.

Related literature

For other methanol/ethanol-coordinated triphenyltin carboxylates, see: Alcock & Roe (1989); Gao *et al.* (2006); Lo & Ng (2009); Ma *et al.* (2004); Ng (1998, 1999); Wang *et al.* (2007); Yeap & Teoh (2003); Yin *et al.* (2002).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_8H_6NO_4)(CH_4O)]$
M_r = 562.17
Monoclinic, $P2_1/n$
a = 10.8385 (13) Å
b = 14.8791 (18) Å
c = 15.8243 (19) Å
β = 94.004 (2)°
V = 2545.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 293 K
0.40 × 0.25 × 0.10 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.681, T_{max} = 0.903
15231 measured reflections
5739 independent reflections
4515 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.08
5739 reflections
313 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C1	2.118 (4)	Sn1—O1	2.146 (2)
Sn1—C7	2.110 (4)	Sn1—O5	2.410 (3)
Sn1—C13	2.121 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O2^{i}	0.85 (1)	1.87 (2)	2.676 (4)	158 (5)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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 Universiti Tunku Abdul Rahman (Vote No. 6200/Y02) and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5330).

References

Alcock, N. W. & Roe, S. M. (1989). *J. Chem. Soc. Dalton Trans.* pp. 1589–1598.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, Z.-J., Yin, H.-D., Li, G. & Xu, H.-L. (2006). *Chin. J. Struct. Chem.* **25**, 1228–1232.
Lo, K. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, m489.
Ma, C.-L., Jiang, Q. & Zhang, Q.-R. (2004). *Can. J. Chem.* **62**, 608–615.
Ng, S. W. (1998). *Acta Cryst.* C**54**, 745–750.
Ng, S. W. (1999). *Acta Cryst.* C**55**, 523–531.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, H.-Y., Yin, H.-D. & Sun, Y.-Y. (2007). *Acta Cryst.* E**63**, m2994.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 43, 920–925.
Yeap, L.-L. & Teoh, S.-G. (2003). *J. Coord. Chem.* **56**, 701–708.
Yin, H.-D., Ma, C.-L., Wang, Y., Fang, H.-X. & Shao, J.-X. (2002). *Acta Chim. Sin.* **60**, 897–903.

supporting information

Acta Cryst. (2010). E**66**, m1164 [https://doi.org/10.1107/S1600536810033623]

(Methanol-κO)(2-methyl-3-nitrobenzoato-κO)triphenyltin(IV)

Foo Win Yip, Siang Guan Teoh, Bohari M. Yamin and Seik Weng Ng

S1. Comment

Triphenyltin(IV) carboxylates generally exist as tetrahedral molecules in which the carboxylate anion is only unidentate to the tin atom. However, there are examples of such compounds having an alcohol molecule into its coordination sphere, as noted in several examples (Alcock & Roe, 1989, Gao *et al.*, 2006; Lo & Ng, 2009; Ma *et al.*, 2004; Ng, 1998; Ng, 1999; Wang *et al.*, 2007; Yeap & Teoh, 2003; Yin *et al.* 2002). The alcohol (either methanol or ethanol) serves as the reaction medium. The condensation of triphenyltin hydroxide and 2-methyl-3-nitrobenzoic acid in methanol gave the expected product as a methanol-coordinated compound (Scheme I, Fig. 1). The five-coordinate tin atom in $Sn(C_6H_5)_3(CH_4O)(C_8H_6NO_4)$ exists in a *trans*-C_3SnO_2 trigonal bipyramidal coordination polyhedron for which the O atoms of the methanol and carboxylate occupy the apical sites. As found in the other examples, the tin-oxygen$_{alcohol}$ bond is longer than the tin-oxygen$_{carboxylate}$ bond (Table 1). However, the C_3Sn girdle is nearly planar [Σ_{angles} 358.6 (5) °]. Adjacent molecules are linked by an O–H···O interaction to generate a helical hydrogen-bonded chain running along the *b*-axis of the monoclinic unit cell (Fig. 2, Table 2).

S2. Experimental

Triphenyltin hydroxide (0.73 g, 2 mmol) and 2-methyl-3-nitrobenzoic acid (0.36 g, 2 mmole) were heated in methanol (50 ml) for an hour. The mixture was filtered to give a clear yellow solution. The filtrate was set aside for the formation of crystals, which were isolated in 80% yield; m.p. 394.5 K. CHN&Sn elemental analysis for $C_{27}H_{25}N_1O_5Sn$: C 57.53, H 4.04, N 2.45, Sn 21.02%. Calc.: C 57.68, H 4.48, N 2.49, Sn 21.11%.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2 to 1.5U(C).

The methanol H-atom was located in a difference Fourier map, and was refined isotropically with a distance restraint of O–H 0.85±0.01 Å.

The final difference Fourier map had two peaks in the vicinity of Sn1.

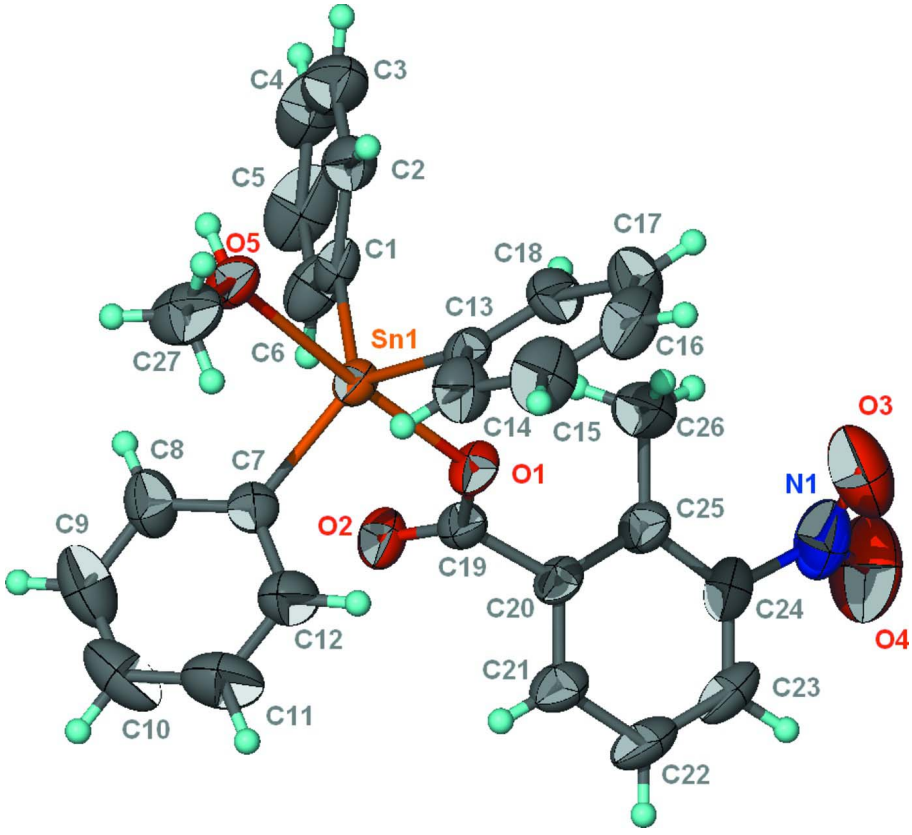


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

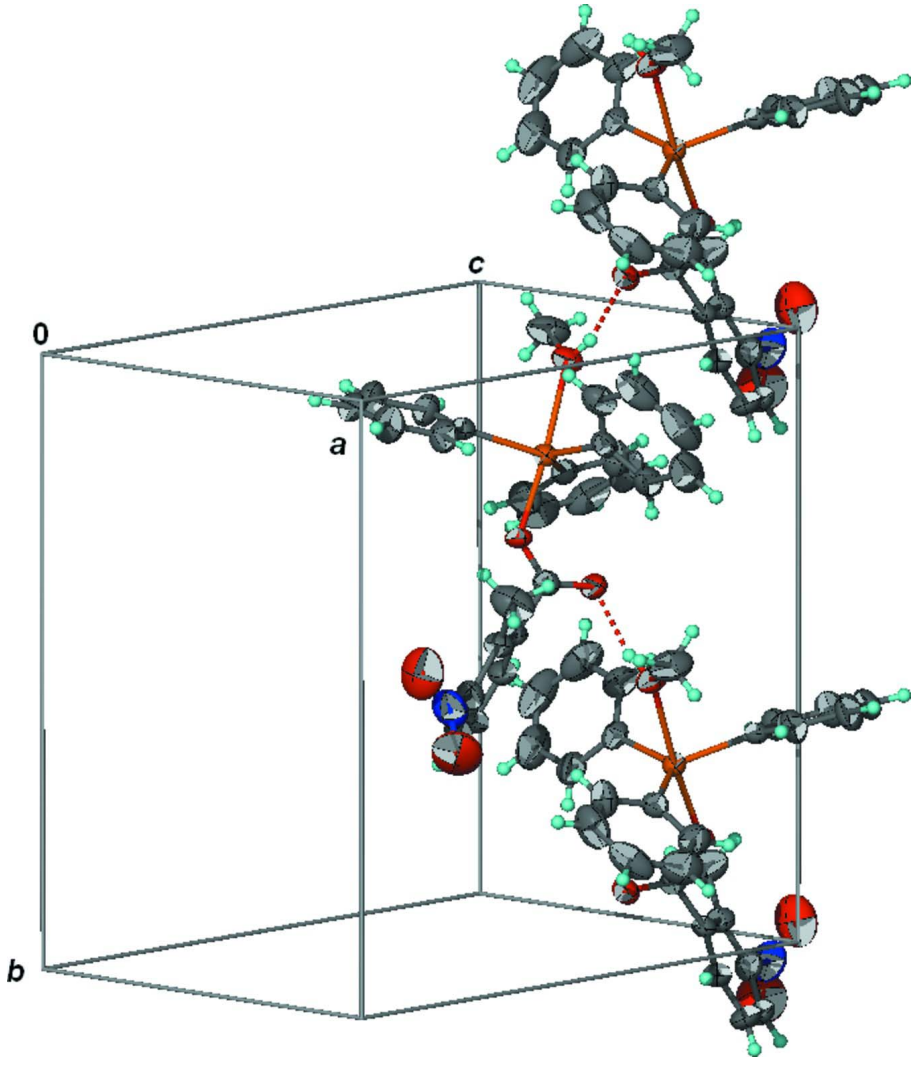


Figure 2

Hydrogen-bonded chain structure.

(Methanol-*κO*)(2-methyl-3-nitrobenzoato-*κO*)triphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_8H_6NO_4)(CH_4O)]$
$M_r = 562.17$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.8385\ (13)$ Å
$b = 14.8791\ (18)$ Å
$c = 15.8243\ (19)$ Å
$\beta = 94.004\ (2)°$
$V = 2545.7\ (5)$ Å^3
$Z = 4$

$F(000) = 1136$
$D_x = 1.467$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 918 reflections
$\theta = 2.7–25.1°$
$\mu = 1.04$ mm^{-1}
$T = 293$ K
Block, yellow
0.40 × 0.25 × 0.10 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.681, T_{max} = 0.903
15231 measured reflections
5739 independent reflections
4515 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −14→13
k = −18→19
l = −20→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.08
5739 reflections
313 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 1.4418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.63268 (2)	0.197738 (16)	0.687848 (16)	0.04465 (10)
O1	0.6379 (3)	0.32447 (16)	0.62345 (18)	0.0566 (7)
O2	0.7358 (3)	0.40787 (19)	0.72344 (18)	0.0635 (7)
O3	0.7290 (6)	0.5035 (5)	0.3367 (3)	0.140 (2)
O4	0.7949 (6)	0.6315 (4)	0.3673 (4)	0.160 (2)
O5	0.6168 (3)	0.05094 (19)	0.7505 (2)	0.0617 (7)
H5	0.679 (3)	0.016 (3)	0.758 (3)	0.089 (17)*
N1	0.7459 (5)	0.5650 (4)	0.3876 (4)	0.0993 (15)
C1	0.8227 (4)	0.1658 (3)	0.6847 (3)	0.0530 (9)
C2	0.8560 (5)	0.0862 (3)	0.6479 (3)	0.0705 (12)
H2	0.7951	0.0485	0.6236	0.085*
C3	0.9784 (7)	0.0619 (5)	0.6469 (4)	0.103 (2)
H3	0.9998	0.0074	0.6231	0.124*
C4	1.0676 (6)	0.1176 (7)	0.6805 (5)	0.118 (3)
H4	1.1502	0.1008	0.6801	0.141*
C5	1.0378 (5)	0.1978 (5)	0.7148 (5)	0.108 (2)
H5A	1.1001	0.2360	0.7368	0.130*
C6	0.9150 (4)	0.2230 (3)	0.7172 (3)	0.0756 (14)
H6	0.8946	0.2780	0.7405	0.091*
C7	0.5464 (4)	0.2443 (3)	0.7950 (2)	0.0512 (9)
C8	0.5951 (5)	0.2284 (4)	0.8764 (3)	0.0766 (13)
H8	0.6674	0.1951	0.8851	0.092*
C9	0.5383 (7)	0.2609 (5)	0.9442 (4)	0.0999 (19)
H9	0.5728	0.2496	0.9986	0.120*

C10	0.4323 (7)	0.3094 (4)	0.9338 (4)	0.101 (2)
H10	0.3944	0.3312	0.9806	0.121*
C11	0.3822 (6)	0.3257 (4)	0.8546 (5)	0.1000 (19)
H11	0.3093	0.3585	0.8471	0.120*
C12	0.4384 (5)	0.2940 (3)	0.7847 (4)	0.0764 (14)
H12	0.4035	0.3061	0.7306	0.092*
C13	0.5186 (3)	0.1510 (2)	0.5826 (2)	0.0473 (8)
C14	0.3968 (4)	0.1301 (3)	0.5878 (3)	0.0704 (12)
H14	0.3631	0.1296	0.6402	0.085*
C15	0.3226 (5)	0.1094 (4)	0.5146 (4)	0.0900 (17)
H15	0.2396	0.0954	0.5187	0.108*
C16	0.3702 (6)	0.1096 (3)	0.4381 (4)	0.0908 (18)
H16	0.3198	0.0972	0.3895	0.109*
C17	0.4918 (7)	0.1280 (4)	0.4322 (3)	0.0914 (17)
H17	0.5257	0.1258	0.3799	0.110*
C18	0.5658 (5)	0.1501 (3)	0.5044 (3)	0.0701 (12)
H18	0.6486	0.1644	0.4997	0.084*
C19	0.6831 (4)	0.3978 (3)	0.6536 (3)	0.0520 (9)
C20	0.6661 (4)	0.4765 (2)	0.5946 (2)	0.0493 (9)
C21	0.5921 (4)	0.5464 (3)	0.6191 (3)	0.0634 (11)
H21	0.5564	0.5429	0.6708	0.076*
C22	0.5704 (5)	0.6205 (3)	0.5691 (4)	0.0773 (15)
H22	0.5198	0.6666	0.5861	0.093*
C23	0.6240 (5)	0.6255 (3)	0.4942 (4)	0.0747 (14)
H23	0.6111	0.6757	0.4597	0.090*
C24	0.6958 (4)	0.5577 (3)	0.4699 (3)	0.0660 (11)
C25	0.7200 (4)	0.4793 (3)	0.5179 (3)	0.0589 (10)
C26	0.8001 (6)	0.4023 (4)	0.4908 (4)	0.0979 (18)
H26	0.8447	0.3771	0.5397	0.147*
H26B	0.8576	0.4242	0.4522	0.147*
H26C	0.7486	0.3569	0.4634	0.147*
C27	0.5104 (5)	0.0158 (4)	0.7849 (4)	0.0936 (18)
H27A	0.5287	0.0021	0.8437	0.140*
H27B	0.4849	−0.0380	0.7550	0.140*
H27C	0.4450	0.0594	0.7794	0.140*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04851 (16)	0.03856 (15)	0.04577 (16)	0.00015 (10)	−0.00464 (10)	0.00265 (10)
O1	0.0819 (19)	0.0289 (12)	0.0569 (16)	−0.0078 (12)	−0.0114 (14)	0.0025 (11)
O2	0.087 (2)	0.0475 (15)	0.0527 (16)	−0.0111 (14)	−0.0160 (15)	0.0024 (13)
O3	0.152 (5)	0.195 (6)	0.075 (3)	−0.012 (4)	0.021 (3)	−0.002 (4)
O4	0.187 (5)	0.158 (5)	0.139 (5)	−0.054 (4)	0.028 (4)	0.063 (4)
O5	0.0636 (18)	0.0493 (15)	0.073 (2)	0.0051 (13)	0.0088 (15)	0.0157 (14)
N1	0.099 (3)	0.111 (4)	0.087 (4)	−0.007 (3)	0.003 (3)	0.037 (3)
C1	0.050 (2)	0.054 (2)	0.055 (2)	0.0003 (17)	0.0007 (17)	0.0189 (19)
C2	0.078 (3)	0.069 (3)	0.066 (3)	0.012 (2)	0.018 (2)	0.012 (2)

C3	0.098 (5)	0.114 (5)	0.103 (5)	0.041 (4)	0.040 (4)	0.027 (4)
C4	0.061 (4)	0.165 (8)	0.130 (6)	0.031 (4)	0.031 (4)	0.067 (6)
C5	0.054 (3)	0.130 (6)	0.140 (6)	−0.019 (3)	−0.005 (3)	0.047 (5)
C6	0.063 (3)	0.069 (3)	0.093 (4)	−0.010 (2)	−0.011 (3)	0.024 (3)
C7	0.056 (2)	0.045 (2)	0.052 (2)	−0.0054 (16)	0.0022 (17)	−0.0023 (17)
C8	0.075 (3)	0.100 (4)	0.053 (3)	−0.004 (3)	−0.007 (2)	−0.002 (3)
C9	0.108 (5)	0.135 (6)	0.056 (3)	−0.030 (4)	0.007 (3)	−0.015 (3)
C10	0.115 (5)	0.104 (5)	0.090 (5)	−0.041 (4)	0.048 (4)	−0.040 (4)
C11	0.085 (4)	0.091 (4)	0.128 (6)	0.008 (3)	0.033 (4)	−0.020 (4)
C12	0.078 (3)	0.077 (3)	0.074 (3)	0.015 (2)	0.006 (3)	−0.005 (2)
C13	0.058 (2)	0.0339 (17)	0.049 (2)	0.0034 (15)	−0.0081 (17)	−0.0018 (15)
C14	0.067 (3)	0.077 (3)	0.066 (3)	−0.015 (2)	−0.010 (2)	−0.003 (2)
C15	0.077 (3)	0.094 (4)	0.095 (4)	−0.026 (3)	−0.024 (3)	−0.001 (3)
C16	0.127 (5)	0.061 (3)	0.077 (4)	−0.014 (3)	−0.044 (4)	−0.006 (3)
C17	0.124 (5)	0.096 (4)	0.052 (3)	0.005 (4)	−0.011 (3)	−0.015 (3)
C18	0.076 (3)	0.076 (3)	0.058 (3)	0.008 (2)	−0.003 (2)	−0.013 (2)
C19	0.059 (2)	0.045 (2)	0.052 (2)	0.0048 (17)	−0.0002 (19)	−0.0010 (17)
C20	0.061 (2)	0.0312 (16)	0.054 (2)	−0.0017 (15)	−0.0105 (18)	−0.0013 (15)
C21	0.072 (3)	0.042 (2)	0.074 (3)	0.0043 (18)	−0.010 (2)	−0.0046 (19)
C22	0.085 (3)	0.042 (2)	0.101 (4)	0.015 (2)	−0.020 (3)	0.002 (2)
C23	0.078 (3)	0.044 (2)	0.097 (4)	0.001 (2)	−0.031 (3)	0.014 (2)
C24	0.071 (3)	0.067 (3)	0.059 (3)	−0.008 (2)	−0.007 (2)	0.015 (2)
C25	0.069 (3)	0.044 (2)	0.062 (3)	0.0004 (18)	0.001 (2)	0.0051 (18)
C26	0.122 (5)	0.088 (4)	0.088 (4)	0.030 (3)	0.039 (4)	0.010 (3)
C27	0.095 (4)	0.065 (3)	0.124 (5)	0.001 (3)	0.034 (4)	0.022 (3)

Geometric parameters (Å, º)

Sn1—C1	2.118 (4)	C11—C12	1.383 (8)
Sn1—C7	2.110 (4)	C11—H11	0.9300
Sn1—C13	2.121 (4)	C12—H12	0.9300
Sn1—O1	2.146 (2)	C13—C18	1.371 (6)
Sn1—O5	2.410 (3)	C13—C14	1.364 (6)
O1—C19	1.275 (5)	C14—C15	1.397 (7)
O2—C19	1.218 (4)	C14—H14	0.9300
O3—N1	1.225 (7)	C15—C16	1.349 (8)
O4—N1	1.179 (6)	C15—H15	0.9300
O5—C27	1.410 (6)	C16—C17	1.356 (9)
O5—H5	0.850 (10)	C16—H16	0.9300
N1—C24	1.450 (7)	C17—C18	1.389 (7)
C1—C6	1.384 (6)	C17—H17	0.9300
C1—C2	1.378 (6)	C18—H18	0.9300
C2—C3	1.376 (8)	C19—C20	1.500 (5)
C2—H2	0.9300	C20—C21	1.385 (5)
C3—C4	1.354 (10)	C20—C25	1.384 (6)
C3—H3	0.9300	C21—C22	1.367 (6)
C4—C5	1.360 (10)	C21—H21	0.9300
C4—H4	0.9300	C22—C23	1.358 (8)

C5—C6	1.386 (8)	C22—H22	0.9300
C5—H5A	0.9300	C23—C24	1.346 (7)
C6—H6	0.9300	C23—H23	0.9300
C7—C8	1.378 (6)	C24—C25	1.407 (6)
C7—C12	1.383 (6)	C25—C26	1.517 (6)
C8—C9	1.363 (8)	C26—H26	0.9600
C8—H8	0.9300	C26—H26B	0.9600
C9—C10	1.357 (9)	C26—H26C	0.9600
C9—H9	0.9300	C27—H27A	0.9600
C10—C11	1.351 (10)	C27—H27B	0.9600
C10—H10	0.9300	C27—H27C	0.9600

C7—Sn1—C1	125.41 (16)	C11—C12—H12	119.8
C7—Sn1—C13	118.16 (15)	C18—C13—C14	118.4 (4)
C1—Sn1—C13	114.98 (16)	C18—C13—Sn1	118.6 (3)
C7—Sn1—O1	96.93 (13)	C14—C13—Sn1	122.7 (3)
C1—Sn1—O1	97.32 (13)	C13—C14—C15	120.2 (5)
C13—Sn1—O1	87.06 (12)	C13—C14—H14	119.9
C7—Sn1—O5	85.35 (13)	C15—C14—H14	119.9
C1—Sn1—O5	84.49 (13)	C16—C15—C14	120.6 (5)
C13—Sn1—O5	88.38 (12)	C16—C15—H15	119.7
O1—Sn1—O5	175.43 (10)	C14—C15—H15	119.7
C19—O1—Sn1	126.7 (3)	C17—C16—C15	119.7 (5)
C27—O5—Sn1	125.3 (3)	C17—C16—H16	120.1
C27—O5—H5	112 (4)	C15—C16—H16	120.1
Sn1—O5—H5	122 (4)	C16—C17—C18	120.0 (6)
O4—N1—O3	119.9 (7)	C16—C17—H17	120.0
O4—N1—C24	120.7 (7)	C18—C17—H17	120.0
O3—N1—C24	119.2 (5)	C13—C18—C17	120.9 (5)
C6—C1—C2	118.8 (4)	C13—C18—H18	119.5
C6—C1—Sn1	122.1 (4)	C17—C18—H18	119.5
C2—C1—Sn1	119.1 (3)	O2—C19—O1	126.0 (4)
C1—C2—C3	120.8 (6)	O2—C19—C20	119.9 (3)
C1—C2—H2	119.6	O1—C19—C20	114.1 (3)
C3—C2—H2	119.6	C21—C20—C25	120.7 (4)
C4—C3—C2	119.8 (6)	C21—C20—C19	117.4 (4)
C4—C3—H3	120.1	C25—C20—C19	121.8 (3)
C2—C3—H3	120.1	C22—C21—C20	121.5 (5)
C5—C4—C3	120.7 (6)	C22—C21—H21	119.2
C5—C4—H4	119.6	C20—C21—H21	119.2
C3—C4—H4	119.6	C21—C22—C23	118.8 (5)
C4—C5—C6	120.3 (6)	C21—C22—H22	120.6
C4—C5—H5A	119.9	C23—C22—H22	120.6
C6—C5—H5A	119.9	C24—C23—C22	120.0 (4)
C1—C6—C5	119.6 (6)	C24—C23—H23	120.0
C1—C6—H6	120.2	C22—C23—H23	120.0
C5—C6—H6	120.2	C23—C24—C25	123.8 (5)
C8—C7—C12	117.8 (4)	C23—C24—N1	117.5 (5)

C8—C7—Sn1	122.1 (3)	C25—C24—N1	118.6 (5)
C12—C7—Sn1	120.0 (3)	C20—C25—C24	115.1 (4)
C9—C8—C7	120.7 (5)	C20—C25—C26	120.7 (4)
C9—C8—H8	119.6	C24—C25—C26	124.2 (4)
C7—C8—H8	119.6	C25—C26—H26	109.5
C8—C9—C10	121.2 (6)	C25—C26—H26B	109.5
C8—C9—H9	119.4	H26—C26—H26B	109.5
C10—C9—H9	119.4	C25—C26—H26C	109.5
C11—C10—C9	119.3 (6)	H26—C26—H26C	109.5
C11—C10—H10	120.3	H26B—C26—H26C	109.5
C9—C10—H10	120.3	O5—C27—H27A	109.5
C10—C11—C12	120.6 (6)	O5—C27—H27B	109.5
C10—C11—H11	119.7	H27A—C27—H27B	109.5
C12—C11—H11	119.7	O5—C27—H27C	109.5
C7—C12—C11	120.3 (6)	H27A—C27—H27C	109.5
C7—C12—H12	119.8	H27B—C27—H27C	109.5

C7—Sn1—O1—C19	53.5 (3)	C1—Sn1—C13—C18	−35.2 (4)
C1—Sn1—O1—C19	−73.7 (3)	O1—Sn1—C13—C18	61.5 (3)
C13—Sn1—O1—C19	171.5 (3)	O5—Sn1—C13—C18	−118.4 (3)
C7—Sn1—O5—C27	46.3 (4)	C7—Sn1—C13—C14	−15.7 (4)
C1—Sn1—O5—C27	172.6 (4)	C1—Sn1—C13—C14	151.3 (3)
C13—Sn1—O5—C27	−72.1 (4)	O1—Sn1—C13—C14	−112.0 (3)
C7—Sn1—C1—C6	−48.3 (4)	O5—Sn1—C13—C14	68.2 (3)
C13—Sn1—C1—C6	145.8 (3)	C18—C13—C14—C15	−0.7 (7)
O1—Sn1—C1—C6	55.7 (4)	Sn1—C13—C14—C15	172.7 (4)
O5—Sn1—C1—C6	−128.6 (4)	C13—C14—C15—C16	0.1 (8)
C7—Sn1—C1—C2	132.7 (3)	C14—C15—C16—C17	1.6 (9)
C13—Sn1—C1—C2	−33.2 (4)	C15—C16—C17—C18	−2.6 (9)
O1—Sn1—C1—C2	−123.4 (3)	C14—C13—C18—C17	−0.3 (7)
O5—Sn1—C1—C2	52.4 (3)	Sn1—C13—C18—C17	−174.1 (4)
C6—C1—C2—C3	2.9 (7)	C16—C17—C18—C13	2.0 (8)
Sn1—C1—C2—C3	−178.1 (4)	Sn1—O1—C19—O2	3.2 (6)
C1—C2—C3—C4	−1.5 (9)	Sn1—O1—C19—C20	−176.5 (3)
C2—C3—C4—C5	−0.5 (10)	O2—C19—C20—C21	−64.5 (5)
C3—C4—C5—C6	1.2 (11)	O1—C19—C20—C21	115.2 (4)
C2—C1—C6—C5	−2.2 (7)	O2—C19—C20—C25	116.6 (5)
Sn1—C1—C6—C5	178.8 (4)	O1—C19—C20—C25	−63.7 (5)
C4—C5—C6—C1	0.2 (9)	C25—C20—C21—C22	−0.5 (6)
C1—Sn1—C7—C8	−23.2 (4)	C19—C20—C21—C22	−179.4 (4)
C13—Sn1—C7—C8	142.3 (4)	C20—C21—C22—C23	−0.7 (7)
O1—Sn1—C7—C8	−127.3 (4)	C21—C22—C23—C24	0.8 (7)
O5—Sn1—C7—C8	56.6 (4)	C22—C23—C24—C25	0.2 (7)
C1—Sn1—C7—C12	155.6 (3)	C22—C23—C24—N1	177.2 (5)
C13—Sn1—C7—C12	−38.8 (4)	O4—N1—C24—C23	48.4 (8)
O1—Sn1—C7—C12	51.5 (4)	O3—N1—C24—C23	−126.4 (6)
O5—Sn1—C7—C12	−124.5 (4)	O4—N1—C24—C25	−134.5 (6)
C12—C7—C8—C9	−0.1 (7)	O3—N1—C24—C25	50.7 (8)

Sn1—C7—C8—C9	178.8 (4)	C21—C20—C25—C24	1.4 (6)
C7—C8—C9—C10	0.3 (9)	C19—C20—C25—C24	−179.7 (4)
C8—C9—C10—C11	0.0 (10)	C21—C20—C25—C26	−179.5 (5)
C9—C10—C11—C12	−0.4 (10)	C19—C20—C25—C26	−0.6 (6)
C8—C7—C12—C11	−0.3 (7)	C23—C24—C25—C20	−1.3 (7)
Sn1—C7—C12—C11	−179.2 (4)	N1—C24—C25—C20	−178.3 (4)
C10—C11—C12—C7	0.6 (9)	C23—C24—C25—C26	179.6 (5)
C7—Sn1—C13—C18	157.8 (3)	N1—C24—C25—C26	2.6 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O2^{i}	0.85 (1)	1.87 (2)	2.676 (4)	158 (5)

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+3/2.