

(2-{[1,1-Bis(hydroxymethyl)-2-oxido-ethyl]iminomethyl}-4-chlorophenolato- $\kappa^3 N,O,O'$)dibutyltin(IV)

Reza Reisi, Misni Misran, Kong Mun Lo and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

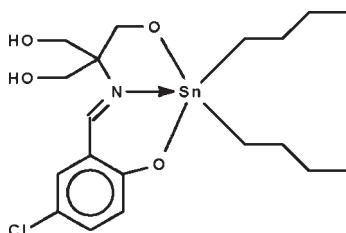
Received 25 March 2010; accepted 25 March 2010

Key indicators: single-crystal X-ray study; $T = 123\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$; R factor = 0.020; wR factor = 0.064; data-to-parameter ratio = 19.8.

The Schiff base ligand in the title compound, $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_{11}\text{H}_{12}\text{ClNO}_4)]$, chelates to the Sn atom through the two deprotonated O atoms, as well as through the N atom, to confer an overall *cis*- C_2SnNO_2 trigonal-bipyramidal geometry at tin [$\text{C}-\text{Sn}-\text{C} = 130.3(1)^\circ$]. The hydroxy groups engage in $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding with the O atoms of adjacent molecules, generating a chain running along the c axis.

Related literature

For the crystal structure of the uncoordinated Schiff base, see: Ng (2008).



Experimental

Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_{11}\text{H}_{12}\text{ClNO}_4)]$	$V = 4184.03(8)\text{ \AA}^3$
$M_r = 490.58$	$Z = 8$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 18.6212(2)\text{ \AA}$	$\mu = 1.37\text{ mm}^{-1}$
$b = 13.4657(2)\text{ \AA}$	$T = 123\text{ K}$
$c = 16.6949(1)\text{ \AA}$	$0.43 \times 0.30 \times 0.25\text{ mm}$
$\beta = 91.845(1)^\circ$	

Data collection

Bruker SMART APEX diffractometer	23501 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	4803 independent reflections
$R_{\text{int}} = 0.025$	4350 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.590$, $T_{\text{max}} = 0.726$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.064$	$\Delta\rho_{\text{max}} = 0.60\text{ e \AA}^{-3}$
$S = 0.94$	$\Delta\rho_{\text{min}} = -0.31\text{ e \AA}^{-3}$
4803 reflections	
243 parameters	
2 restraints	

Table 1
Selected geometric parameters (\AA , $^\circ$).

Sn1—O1	2.118 (1)	Sn1—C5	2.136 (2)
Sn1—O2	2.106 (1)	Sn1—N1	2.215 (1)
Sn1—C1	2.136 (2)		
C1—Sn1—C5	130.26 (8)		

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

D—H \cdots A	D—H	H \cdots A	D \cdots A	D—H \cdots A
O3—H3o \cdots O2 ⁱ	0.83 (1)	1.79 (1)	2.612 (2)	172 (3)
O4—H4o \cdots O3 ⁱⁱ	0.84 (1)	1.94 (1)	2.739 (2)	160 (2)

Symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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 the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5229).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
- Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Ng, S. W. (2008). *Acta Cryst. E* **64**, o2455.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Westrip, S. P. (2010). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2010). E66, m482 [doi:10.1107/S1600536810011384]

(2-{[1,1-Bis(hydroxymethyl)-2-oxidoethyl]iminomethyl}-4-chlorophenolato- κ^3N,O,O')dibutyltin(IV)

R. Reisi, M. Misran, K. M. Lo and S. W. Ng

Comment

The Schiff base derived from the condensation of salicylaldehyde (and other substituted salicyldehydes) and tris(hydroxymethyl)methylamine is invariably deprotonated with respect to the phenoxy hydrogen atom and the deprotonated ligand binds to a metal atom through this oxygen atom. Occasionally, one of the methylelenehydroxy groups is also deprotonated in the metal complexes. The 4-chloro substituted compound, which exists as a zwitterion (Ng, 2008), when reacted with dibutyltin oxide is doubly-deprotonated in order to balance the charge of tin so that the ligand binds in a terdentate manner (Scheme I, Fig. 1).

The tin atom shows *cis*-trigonal bipyramidal coordination with a C–Sn–C angle of 130.3 (1)°; the ligand spans the two axial sites. The C–Sn–C angle is not opened up by the electronegative atom of any adjacent molecule. Adjacent molecules are linked by hydrogen bonds to form a ribbon (Fig. 2).

Experimental

The Schiff base, 4-chloro-2-tris[(hydroxymethyl)methylimino]phenol was prepared from *tris*(hydroxymethyl)aminomethane and 5-chlorosalicylaldehyde in ethanol. The compound (0.26 g, 0.1 mmol) and dibutyltin oxide (0.25 g, 1.0 mmol) were heated in toluene in a Dean-Stark apparatus for 8 hours. Crystals were obtained when the filtered solution was allowed to evaporate over several days.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 to 1.5 $U(C)$.

The hydroxy H-atoms were located in a difference Fourier map, and were refined isotropically with a distance restraint of O—H 0.84±0.01 Å.

Figures

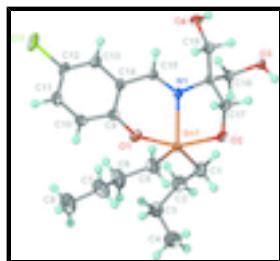


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_{11}\text{H}_{12}\text{ClNO}_4)$ with ellipsoids at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

supplementary materials

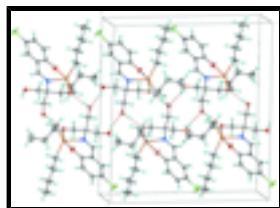


Fig. 2. Packing diagram of the title compound.

(2-{{[1,1-Bis(hydroxymethyl)-2-oxidoethyl]iminomethyl}-4-chlorophenolato- κ^3N,O,O' }dibutyltin(IV)

Crystal data

[Sn(C ₄ H ₉) ₂ (C ₁₁ H ₁₂ ClNO ₄)]	$F(000) = 2000$
$M_r = 490.58$	$D_x = 1.558 \text{ Mg m}^{-3}$
Monoclinic, C2/c	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -C 2yc	Cell parameters from 9381 reflections
$a = 18.6212 (2) \text{ \AA}$	$\theta = 2.2\text{--}31.7^\circ$
$b = 13.4657 (2) \text{ \AA}$	$\mu = 1.37 \text{ mm}^{-1}$
$c = 16.6949 (1) \text{ \AA}$	$T = 123 \text{ K}$
$\beta = 91.845 (1)^\circ$	Block, yellow
$V = 4184.03 (8) \text{ \AA}^3$	$0.43 \times 0.30 \times 0.25 \text{ mm}$
$Z = 8$	

Data collection

Bruker SMART APEX diffractometer	4803 independent reflections
Radiation source: fine-focus sealed tube graphite	4350 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.025$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 3.0^\circ$
$T_{\text{min}} = 0.590, T_{\text{max}} = 0.726$	$h = -24 \rightarrow 24$
23501 measured reflections	$k = -15 \rightarrow 17$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.020$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.064$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.94$	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 2.5005P]$ where $P = (F_o^2 + 2F_c^2)/3$
4803 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
243 parameters	$\Delta\rho_{\text{max}} = 0.60 \text{ e \AA}^{-3}$

2 restraints

$$\Delta\rho_{\min} = -0.31 \text{ e \AA}^{-3}$$

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	0.324176 (5)	0.374067 (8)	0.254047 (6)	0.01818 (5)
C11	0.05353 (3)	0.31243 (4)	-0.07291 (3)	0.03821 (13)
N1	0.33156 (7)	0.43789 (10)	0.13234 (8)	0.0169 (3)
O1	0.26803 (7)	0.26136 (9)	0.18945 (7)	0.0251 (3)
O2	0.39660 (6)	0.49305 (9)	0.27014 (7)	0.0213 (2)
O3	0.51910 (6)	0.51554 (9)	0.10309 (7)	0.0208 (2)
O4	0.37037 (6)	0.56261 (10)	-0.01897 (7)	0.0233 (3)
C1	0.40248 (10)	0.27086 (14)	0.29943 (12)	0.0280 (4)
H1A	0.4452	0.2757	0.2658	0.034*
H1B	0.4175	0.2922	0.3542	0.034*
C2	0.38064 (11)	0.16181 (15)	0.30333 (12)	0.0318 (4)
H2A	0.3669	0.1391	0.2486	0.038*
H2B	0.4229	0.1224	0.3218	0.038*
C3	0.31878 (12)	0.14046 (16)	0.35828 (14)	0.0367 (5)
H3A	0.2761	0.1786	0.3392	0.044*
H3B	0.3066	0.0690	0.3546	0.044*
C4	0.33487 (16)	0.1662 (3)	0.44466 (15)	0.0629 (8)
H4A	0.2930	0.1507	0.4765	0.094*
H4B	0.3458	0.2372	0.4492	0.094*
H4C	0.3763	0.1276	0.4646	0.094*
C5	0.23412 (10)	0.43890 (15)	0.31046 (12)	0.0298 (4)
H5A	0.2499	0.4597	0.3651	0.036*
H5B	0.2204	0.4997	0.2804	0.036*
C6	0.16740 (12)	0.37495 (16)	0.31741 (16)	0.0403 (5)
H6A	0.1547	0.3469	0.2640	0.048*
H6B	0.1789	0.3187	0.3538	0.048*
C7	0.10287 (11)	0.42862 (17)	0.34800 (15)	0.0420 (5)
H7A	0.0889	0.4814	0.3092	0.050*
H7B	0.1168	0.4614	0.3993	0.050*
C8	0.03807 (14)	0.3637 (2)	0.36135 (19)	0.0559 (7)
H8A	-0.0008	0.4042	0.3822	0.084*
H8B	0.0509	0.3114	0.4000	0.084*
H8C	0.0221	0.3334	0.3104	0.084*
C9	0.22124 (9)	0.27459 (12)	0.12977 (9)	0.0194 (3)
C10	0.16258 (9)	0.20867 (13)	0.11998 (10)	0.0236 (3)
H10	0.1584	0.1544	0.1559	0.028*
C11	0.11135 (9)	0.22152 (14)	0.05944 (10)	0.0245 (4)
H11	0.0710	0.1785	0.0557	0.029*
C12	0.11877 (9)	0.29764 (13)	0.00376 (10)	0.0230 (3)
C13	0.17673 (10)	0.36033 (13)	0.00828 (11)	0.0229 (4)
H13	0.1826	0.4098	-0.0315	0.028*
C14	0.22784 (8)	0.35110 (13)	0.07241 (10)	0.0186 (3)
C15	0.28649 (8)	0.42135 (12)	0.07342 (10)	0.0181 (3)

supplementary materials

H15	0.2925	0.4591	0.0261	0.022*
C16	0.38984 (8)	0.51236 (12)	0.12515 (9)	0.0159 (3)
C17	0.39581 (9)	0.56345 (12)	0.20768 (9)	0.0192 (3)
H17A	0.4404	0.6034	0.2112	0.023*
H17B	0.3546	0.6090	0.2136	0.023*
C18	0.45807 (8)	0.45272 (12)	0.10880 (10)	0.0180 (3)
H18A	0.4667	0.4042	0.1526	0.022*
H18B	0.4510	0.4152	0.0581	0.022*
C19	0.37587 (9)	0.59373 (13)	0.06223 (10)	0.0201 (3)
H19B	0.3307	0.6282	0.0752	0.024*
H19A	0.4152	0.6431	0.0674	0.024*
H3O	0.5441 (11)	0.5129 (19)	0.1452 (9)	0.043 (7)*
H4O	0.4099 (8)	0.5403 (17)	-0.0338 (13)	0.036 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01691 (8)	0.02207 (8)	0.01539 (8)	-0.00301 (4)	-0.00201 (5)	0.00291 (4)
Cl1	0.0319 (2)	0.0357 (3)	0.0454 (3)	-0.00971 (19)	-0.0231 (2)	0.0064 (2)
N1	0.0143 (6)	0.0188 (7)	0.0176 (6)	-0.0016 (5)	0.0002 (5)	0.0011 (5)
O1	0.0287 (6)	0.0245 (6)	0.0215 (6)	-0.0075 (5)	-0.0081 (5)	0.0056 (5)
O2	0.0235 (6)	0.0246 (6)	0.0157 (5)	-0.0051 (5)	-0.0039 (4)	0.0021 (5)
O3	0.0147 (5)	0.0293 (7)	0.0184 (6)	-0.0050 (4)	-0.0022 (4)	0.0037 (5)
O4	0.0210 (6)	0.0322 (7)	0.0165 (6)	0.0003 (5)	0.0003 (5)	0.0036 (5)
C1	0.0220 (8)	0.0282 (10)	0.0334 (10)	-0.0012 (7)	-0.0055 (7)	0.0062 (8)
C2	0.0328 (10)	0.0266 (10)	0.0355 (10)	0.0011 (8)	-0.0034 (8)	0.0027 (8)
C3	0.0356 (11)	0.0367 (11)	0.0372 (12)	-0.0116 (8)	-0.0060 (9)	0.0108 (9)
C4	0.0592 (17)	0.094 (2)	0.0357 (13)	-0.0296 (16)	-0.0015 (12)	0.0084 (14)
C5	0.0264 (9)	0.0296 (10)	0.0337 (10)	-0.0011 (7)	0.0066 (7)	-0.0002 (8)
C6	0.0269 (10)	0.0461 (14)	0.0485 (14)	-0.0077 (8)	0.0097 (9)	-0.0149 (10)
C7	0.0303 (10)	0.0395 (12)	0.0570 (14)	0.0044 (9)	0.0120 (10)	0.0132 (10)
C8	0.0296 (12)	0.080 (2)	0.0587 (17)	-0.0080 (11)	0.0091 (11)	-0.0029 (13)
C9	0.0205 (8)	0.0202 (8)	0.0173 (7)	-0.0016 (6)	-0.0003 (6)	-0.0012 (6)
C10	0.0286 (9)	0.0232 (9)	0.0189 (8)	-0.0089 (7)	0.0012 (7)	0.0012 (6)
C11	0.0208 (8)	0.0274 (9)	0.0252 (9)	-0.0083 (7)	0.0013 (6)	-0.0056 (7)
C12	0.0197 (8)	0.0246 (9)	0.0242 (8)	-0.0015 (6)	-0.0067 (6)	-0.0025 (7)
C13	0.0225 (8)	0.0224 (9)	0.0234 (9)	-0.0034 (6)	-0.0059 (7)	0.0036 (6)
C14	0.0166 (7)	0.0208 (8)	0.0183 (8)	-0.0017 (6)	-0.0020 (6)	-0.0001 (6)
C15	0.0175 (7)	0.0197 (8)	0.0170 (7)	-0.0016 (6)	-0.0004 (6)	0.0023 (6)
C16	0.0144 (7)	0.0174 (8)	0.0159 (7)	-0.0027 (5)	-0.0014 (5)	0.0000 (6)
C17	0.0222 (8)	0.0188 (8)	0.0165 (7)	-0.0009 (6)	0.0000 (6)	-0.0010 (6)
C18	0.0165 (7)	0.0183 (8)	0.0191 (7)	-0.0018 (6)	-0.0008 (6)	0.0004 (6)
C19	0.0213 (8)	0.0197 (8)	0.0191 (8)	0.0003 (6)	-0.0011 (6)	0.0025 (6)

Geometric parameters (\AA , $^\circ$)

Sn1—O1	2.118 (1)	C6—C7	1.506 (3)
Sn1—O2	2.106 (1)	C6—H6A	0.9900
Sn1—C1	2.136 (2)	C6—H6B	0.9900

Sn1—C5	2.136 (2)	C7—C8	1.513 (3)
Sn1—N1	2.215 (1)	C7—H7A	0.9900
C11—C12	1.7476 (17)	C7—H7B	0.9900
N1—C15	1.292 (2)	C8—H8A	0.9800
N1—C16	1.4852 (19)	C8—H8B	0.9800
O1—C9	1.314 (2)	C8—H8C	0.9800
O2—C17	1.4091 (19)	C9—C10	1.413 (2)
O3—C18	1.4224 (18)	C9—C14	1.415 (2)
O3—H3O	0.831 (10)	C10—C11	1.378 (2)
O4—C19	1.419 (2)	C10—H10	0.9500
O4—H4O	0.840 (10)	C11—C12	1.394 (3)
C1—C2	1.526 (3)	C11—H11	0.9500
C1—H1A	0.9900	C12—C13	1.370 (2)
C1—H1B	0.9900	C13—C14	1.415 (2)
C2—C3	1.523 (3)	C13—H13	0.9500
C2—H2A	0.9900	C14—C15	1.445 (2)
C2—H2B	0.9900	C15—H15	0.9500
C3—C4	1.504 (3)	C16—C19	1.534 (2)
C3—H3A	0.9900	C16—C18	1.535 (2)
C3—H3B	0.9900	C16—C17	1.541 (2)
C4—H4A	0.9800	C17—H17A	0.9900
C4—H4B	0.9800	C17—H17B	0.9900
C4—H4C	0.9800	C18—H18A	0.9900
C5—C6	1.519 (3)	C18—H18B	0.9900
C5—H5A	0.9900	C19—H19B	0.9900
C5—H5B	0.9900	C19—H19A	0.9900
O2—Sn1—O1	156.02 (5)	C8—C7—H7A	108.5
O2—Sn1—C1	91.30 (6)	C6—C7—H7B	108.5
O1—Sn1—C1	91.98 (6)	C8—C7—H7B	108.5
O2—Sn1—C5	98.13 (6)	H7A—C7—H7B	107.5
O1—Sn1—C5	97.80 (6)	C7—C8—H8A	109.5
C1—Sn1—C5	130.26 (8)	C7—C8—H8B	109.5
O2—Sn1—N1	76.31 (5)	H8A—C8—H8B	109.5
O1—Sn1—N1	81.67 (5)	C7—C8—H8C	109.5
C1—Sn1—N1	121.08 (6)	H8A—C8—H8C	109.5
C5—Sn1—N1	108.59 (7)	H8B—C8—H8C	109.5
C15—N1—C16	120.89 (13)	O1—C9—C10	119.58 (15)
C15—N1—Sn1	125.01 (11)	O1—C9—C14	122.82 (14)
C16—N1—Sn1	113.79 (9)	C10—C9—C14	117.57 (14)
C9—O1—Sn1	126.37 (11)	C11—C10—C9	121.35 (16)
C17—O2—Sn1	115.22 (9)	C11—C10—H10	119.3
C18—O3—H3O	110.1 (17)	C9—C10—H10	119.3
C19—O4—H4O	110.5 (16)	C10—C11—C12	120.03 (15)
C2—C1—Sn1	117.49 (12)	C10—C11—H11	120.0
C2—C1—H1A	107.9	C12—C11—H11	120.0
Sn1—C1—H1A	107.9	C13—C12—C11	120.74 (15)
C2—C1—H1B	107.9	C13—C12—C11	119.85 (14)
Sn1—C1—H1B	107.9	C11—C12—C11	119.40 (13)
H1A—C1—H1B	107.2	C12—C13—C14	119.79 (16)

supplementary materials

C3—C2—C1	114.53 (17)	C12—C13—H13	120.1
C3—C2—H2A	108.6	C14—C13—H13	120.1
C1—C2—H2A	108.6	C9—C14—C13	120.36 (15)
C3—C2—H2B	108.6	C9—C14—C15	123.44 (14)
C1—C2—H2B	108.6	C13—C14—C15	116.18 (15)
H2A—C2—H2B	107.6	N1—C15—C14	126.46 (15)
C4—C3—C2	113.76 (19)	N1—C15—H15	116.8
C4—C3—H3A	108.8	C14—C15—H15	116.8
C2—C3—H3A	108.8	N1—C16—C19	115.43 (12)
C4—C3—H3B	108.8	N1—C16—C18	105.80 (12)
C2—C3—H3B	108.8	C19—C16—C18	112.02 (13)
H3A—C3—H3B	107.7	N1—C16—C17	105.13 (12)
C3—C4—H4A	109.5	C19—C16—C17	107.40 (13)
C3—C4—H4B	109.5	C18—C16—C17	110.87 (12)
H4A—C4—H4B	109.5	O2—C17—C16	111.11 (13)
C3—C4—H4C	109.5	O2—C17—H17A	109.4
H4A—C4—H4C	109.5	C16—C17—H17A	109.4
H4B—C4—H4C	109.5	O2—C17—H17B	109.4
C6—C5—Sn1	117.23 (14)	C16—C17—H17B	109.4
C6—C5—H5A	108.0	H17A—C17—H17B	108.0
Sn1—C5—H5A	108.0	O3—C18—C16	111.62 (13)
C6—C5—H5B	108.0	O3—C18—H18A	109.3
Sn1—C5—H5B	108.0	C16—C18—H18A	109.3
H5A—C5—H5B	107.2	O3—C18—H18B	109.3
C7—C6—C5	114.67 (17)	C16—C18—H18B	109.3
C7—C6—H6A	108.6	H18A—C18—H18B	108.0
C5—C6—H6A	108.6	O4—C19—C16	116.64 (14)
C7—C6—H6B	108.6	O4—C19—H19B	108.1
C5—C6—H6B	108.6	C16—C19—H19B	108.1
H6A—C6—H6B	107.6	O4—C19—H19A	108.1
C6—C7—C8	114.9 (2)	C16—C19—H19A	108.1
C6—C7—H7A	108.5	H19B—C19—H19A	107.3
O2—Sn1—N1—C15	-163.22 (14)	C9—C10—C11—C12	3.4 (3)
O1—Sn1—N1—C15	26.37 (13)	C10—C11—C12—C13	0.1 (3)
C1—Sn1—N1—C15	113.65 (14)	C10—C11—C12—Cl1	179.67 (14)
C5—Sn1—N1—C15	-69.11 (15)	C11—C12—C13—C14	-3.2 (3)
O2—Sn1—N1—C16	10.39 (10)	Cl1—C12—C13—C14	177.18 (14)
O1—Sn1—N1—C16	-160.03 (11)	O1—C9—C14—C13	178.46 (16)
C1—Sn1—N1—C16	-72.75 (12)	C10—C9—C14—C13	0.4 (2)
C5—Sn1—N1—C16	104.50 (11)	O1—C9—C14—C15	0.4 (3)
O2—Sn1—O1—C9	-64.26 (19)	C10—C9—C14—C15	-177.68 (16)
C1—Sn1—O1—C9	-161.94 (14)	C12—C13—C14—C9	3.0 (3)
C5—Sn1—O1—C9	66.95 (14)	C12—C13—C14—C15	-178.85 (16)
N1—Sn1—O1—C9	-40.81 (13)	C16—N1—C15—C14	179.74 (15)
O1—Sn1—O2—C17	41.07 (18)	Sn1—N1—C15—C14	-7.1 (2)
C1—Sn1—O2—C17	138.89 (12)	C9—C14—C15—N1	-14.7 (3)
C5—Sn1—O2—C17	-90.09 (12)	C13—C14—C15—N1	167.15 (17)
N1—Sn1—O2—C17	17.16 (10)	C15—N1—C16—C19	23.6 (2)
O2—Sn1—C1—C2	-179.95 (15)	Sn1—N1—C16—C19	-150.32 (11)

O1—Sn1—C1—C2	−23.71 (15)	C15—N1—C16—C18	−100.89 (16)
C5—Sn1—C1—C2	78.25 (18)	Sn1—N1—C16—C18	85.21 (12)
N1—Sn1—C1—C2	−105.17 (15)	C15—N1—C16—C17	141.72 (15)
Sn1—C1—C2—C3	−62.2 (2)	Sn1—N1—C16—C17	−32.18 (14)
C1—C2—C3—C4	−61.8 (3)	Sn1—O2—C17—C16	−41.23 (15)
O2—Sn1—C5—C6	−176.69 (16)	N1—C16—C17—O2	46.68 (16)
O1—Sn1—C5—C6	21.30 (17)	C19—C16—C17—O2	170.11 (12)
C1—Sn1—C5—C6	−78.01 (19)	C18—C16—C17—O2	−67.21 (16)
N1—Sn1—C5—C6	105.09 (17)	N1—C16—C18—O3	−178.13 (12)
Sn1—C5—C6—C7	−172.58 (17)	C19—C16—C18—O3	55.30 (17)
C5—C6—C7—C8	−175.3 (2)	C17—C16—C18—O3	−64.66 (16)
Sn1—O1—C9—C10	−146.41 (13)	N1—C16—C19—O4	−64.69 (18)
Sn1—O1—C9—C14	35.5 (2)	C18—C16—C19—O4	56.47 (18)
O1—C9—C10—C11	178.29 (16)	C17—C16—C19—O4	178.44 (13)
C14—C9—C10—C11	−3.5 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O3—H3o···O2 ⁱ	0.83 (1)	1.79 (1)	2.612 (2)	172 (3)
O4—H4o···O3 ⁱⁱ	0.84 (1)	1.94 (1)	2.739 (2)	160 (2)

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

supplementary materials

Fig. 1

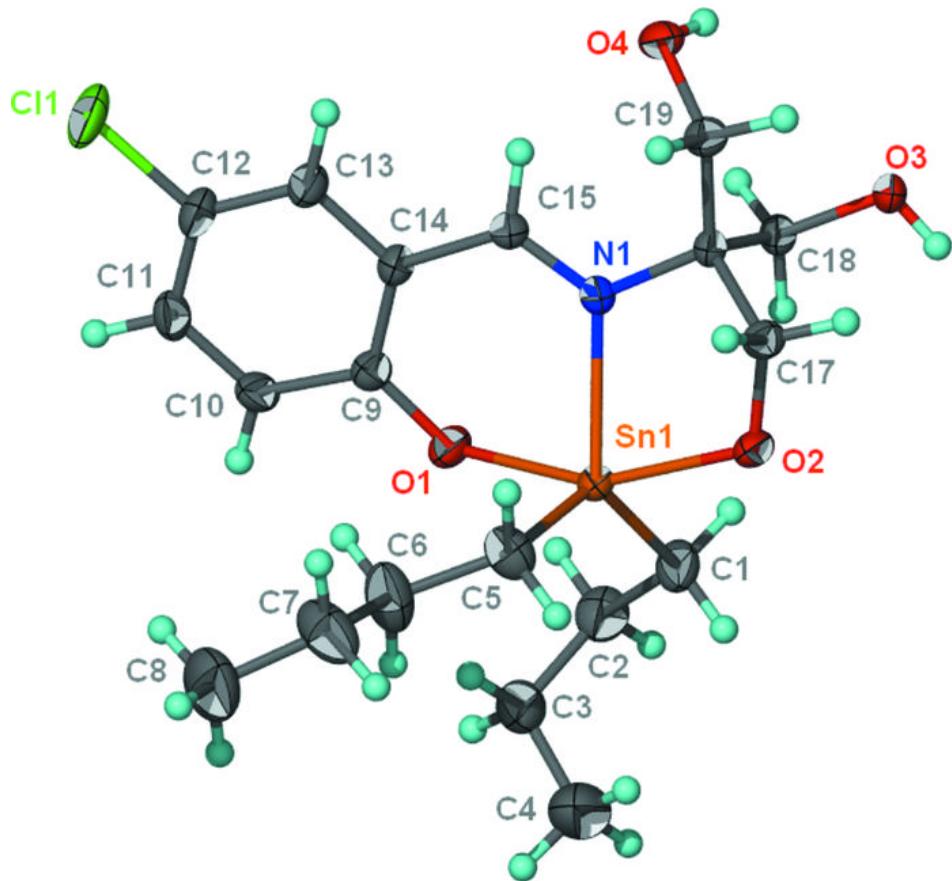


Fig. 2

