

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

See Mun Lee, Hapipah Mohd Ali and Kong Mun Lo*

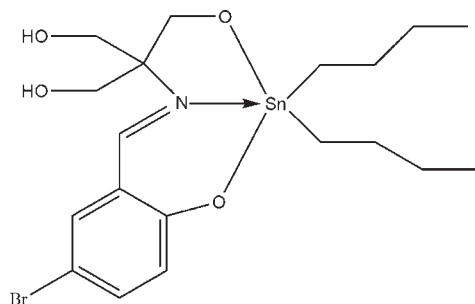
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.022; wR factor = 0.052; data-to-parameter ratio = 20.0.

In the title compound, $[Sn(C_4H_9)_2(C_{11}H_{12}BrNO_4)]$, the Schiff base ligand chelates to the Sn^{IV} atom through the two deprotonated hydroxy groups, as well as through the N atom, to confer an overall *cis*- C_2SnNO_2 trigonal-bipyramidal geometry at the Sn^{IV} atom [$C-Sn-C = 129.92(9)^\circ$]. The remaining methylenehydroxy groups engage in $O-H \cdots O$ hydrogen bonding with the O atoms of adjacent molecules, leading to infinite supramolecular chains propagating in $[001]$.

Related literature

 For related structures, see Reisi *et al.* (2010); Ng (2008).


Experimental

Crystal data

| | |
|--------------------------------------|--------------------------------|
| $[Sn(C_4H_9)_2(C_{11}H_{12}BrNO_4)]$ | $b = 13.3811(7)$ Å |
| $M_r = 535.04$ | $c = 16.5768(8)$ Å |
| Monoclinic, $C2/c$ | $\beta = 91.385(3)^\circ$ |
| $a = 18.8326(9)$ Å | $V = 4176.1(4)$ Å ³ |

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 3.16$ mm⁻¹

$T = 100$ K
 $0.40 \times 0.10 \times 0.08$ mm

Data collection

| | |
|--|--|
| Bruker APEXII CCD area-detector diffractometer | 19535 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2009) | 4785 independent reflections |
| $T_{min} = 0.365$, $T_{max} = 0.786$ | 4229 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.032$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.022$ | 2 restraints |
| $wR(F^2) = 0.052$ | H-atom parameters constrained |
| $S = 1.02$ | $\Delta\rho_{max} = 0.65$ e Å ⁻³ |
| 4785 reflections | $\Delta\rho_{min} = -0.38$ e Å ⁻³ |
| 239 parameters | |

Table 1
 Selected bond lengths (Å).

| | | | |
|--------|-------------|---------|-----------|
| Sn1—N1 | 2.2108 (17) | Sn1—C12 | 2.139 (2) |
| Sn1—O1 | 2.1203 (15) | Sn1—C16 | 2.129 (2) |
| Sn1—O2 | 2.1049 (14) | | |

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

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|------------------------|-------|--------------|--------------|----------------|
| $O3-H3 \cdots O2^i$ | 0.84 | 1.77 | 2.608 (2) | 174 |
| $O4-H4 \cdots O3^{ii}$ | 0.84 | 1.93 | 2.733 (2) | 160 |

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

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: pubCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2772).

References

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supporting information

Acta Cryst. (2010). E66, m793 [doi:10.1107/S1600536810021872]

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

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S1. Comment

The Schiff base derived from the condensation of 5-bromosalicylaldehyde and tris(hydroxymethyl)methylamine is deprotonated with respect to the phenoxy hydrogen atom and one of the methylenehydroxyl hydrogen atom. The ligand coordinates to the dibutyltin fragment through this doubly deprotonated oxygen atoms and the imine nitrogen (Fig. 1).

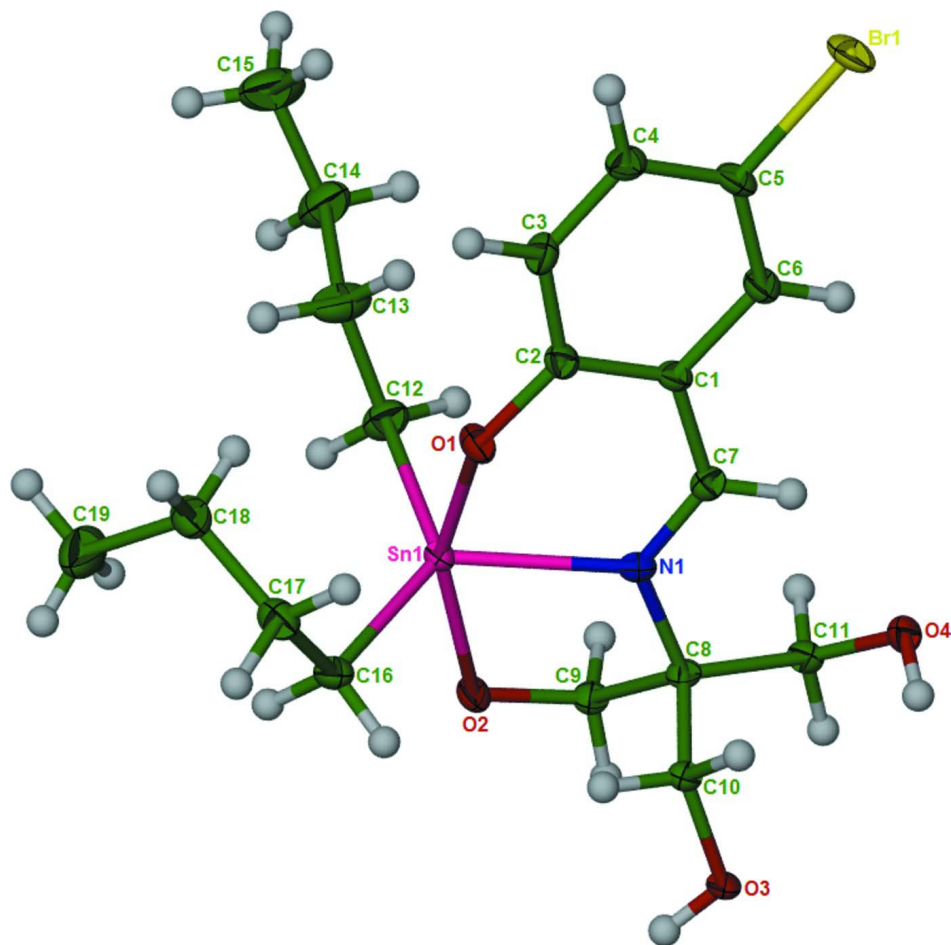
The tin atom is in a *cis*-trigonal bipyramidal geometry with a C—Sn—C angle of 129.92 (9)°. The two deprotonated oxygen atoms occupied the axial sites with a O—Sn—O angle of 155.60 (6)°, indicating a distortion in the trigonal bipyramidal geometry at the Sn atom. Adjacent molecules are linked by hydrogen bonds to form an infinite polymeric chain (Fig. 2).

S2. Experimental

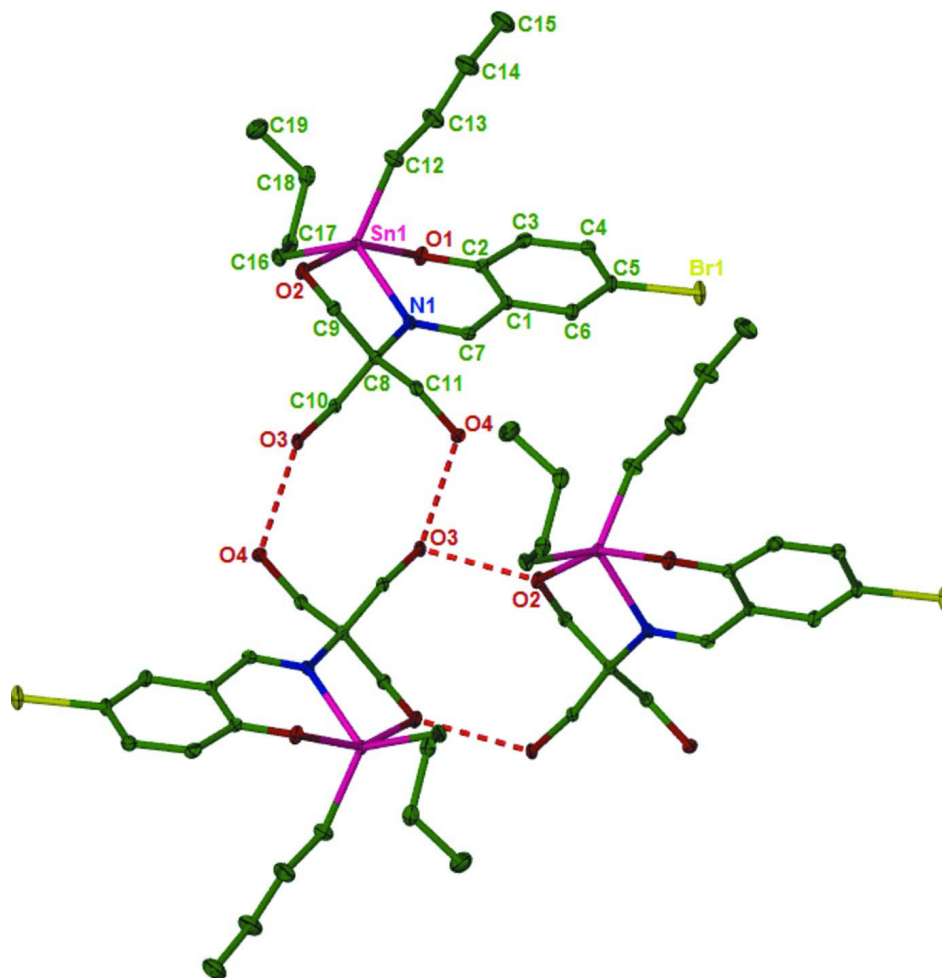
The Schiff base, 4-bromo-2-tris[(hydroxymethyl)methylimino]phenol was prepared from tris(hydroxymethyl)amino-methane and 5-bromosalicylaldehyde in absolute ethanol. The compound (0.30 g, 0.1 mmol) and dibutyltin oxide (0.25 g, 1.0 mmol) were heated in 50 ml of toluene in a Dean-Stark apparatus for 8 h. The solution was left for crystallization for a week during which yellow crystals were obtained.

S3. Refinement

Hydrogen atoms were placed at calculated positions (C—H 0.95 to 0.98 Å) and were treated as riding on their parent carbon atoms, with $U_{\text{iso}}(\text{H})$ set to 1.2–1.5 times $U_{\text{eq}}(\text{C})$. The hydroxy-H was refined with a restraint of 0.84 ± 0.01 Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The molecular structure of (2-([1,1-bis(hydroxymethyl)-2-oxidoethyl]iminomethyl)-4-chlorophenolato- κ^3N,O,O')dibutyltin(IV) showing 70% probability displacement ellipsoids and the atom numbering. Hydrogen atoms are drawn as spheres of arbitrary radius.

**Figure 2**

Crystal packing of the unit cell showing the hydrogen bonding interactions in the molecule.

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

Crystal data

[Sn(C₄H₉)₂(C₁₁H₁₂BrNO₄)]

$M_r = 535.04$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 18.8326$ (9) Å

$b = 13.3811$ (7) Å

$c = 16.5768$ (8) Å

$\beta = 91.385$ (3)°

$V = 4176.1$ (4) Å³

$Z = 8$

$F(000) = 2144$

$D_x = 1.702$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7855 reflections

$\theta = 2.2$ – 30.4 °

$\mu = 3.16$ mm⁻¹

$T = 100$ K

Needle, yellow

$0.40 \times 0.10 \times 0.08$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube
Graphite monochromator

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.365$, $T_{\max} = 0.786$

19535 measured reflections
 4785 independent reflections
 4229 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.9^\circ$
 $h = -24 \rightarrow 24$
 $k = -17 \rightarrow 17$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.052$
 $S = 1.02$
 4785 reflections
 239 parameters
 2 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 4.784P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.65 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$

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.

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|----------------|----------------------------------|
| Sn1 | 0.325854 (7) | 0.128538 (10) | 0.254101 (8) | 0.01133 (5) |
| Br1 | 0.047899 (12) | 0.180095 (17) | -0.072373 (14) | 0.02090 (6) |
| N1 | 0.33348 (9) | 0.06301 (13) | 0.13219 (10) | 0.0117 (3) |
| O1 | 0.27217 (8) | 0.24249 (11) | 0.18796 (9) | 0.0154 (3) |
| O2 | 0.39697 (8) | 0.00855 (11) | 0.27086 (8) | 0.0141 (3) |
| O3 | 0.51910 (7) | -0.01628 (11) | 0.10327 (9) | 0.0139 (3) |
| H3 | 0.5442 | -0.0111 | 0.1456 | 0.021* |
| O4 | 0.37130 (8) | -0.06319 (12) | -0.01932 (8) | 0.0151 (3) |
| H4 | 0.4107 | -0.0416 | -0.0344 | 0.023* |
| C1 | 0.22983 (11) | 0.14839 (15) | 0.07343 (12) | 0.0119 (4) |
| C2 | 0.22471 (11) | 0.22806 (16) | 0.12949 (12) | 0.0132 (4) |
| C3 | 0.16695 (12) | 0.29422 (16) | 0.12036 (12) | 0.0153 (4) |
| H3A | 0.1638 | 0.3502 | 0.1554 | 0.018* |
| C4 | 0.11478 (11) | 0.27967 (17) | 0.06175 (13) | 0.0155 (4) |
| H4A | 0.0751 | 0.3234 | 0.0581 | 0.019* |
| C5 | 0.12066 (11) | 0.19991 (16) | 0.00753 (12) | 0.0148 (4) |
| C6 | 0.17791 (11) | 0.13705 (16) | 0.01159 (13) | 0.0144 (4) |
| H6 | 0.1826 | 0.0856 | -0.0274 | 0.017* |
| C7 | 0.28804 (11) | 0.07801 (16) | 0.07408 (12) | 0.0125 (4) |
| H7 | 0.2933 | 0.0388 | 0.0268 | 0.015* |
| C8 | 0.39114 (11) | -0.01213 (15) | 0.12512 (12) | 0.0116 (4) |

| | | | | |
|------|--------------|---------------|--------------|------------|
| C9 | 0.39651 (11) | -0.06281 (16) | 0.20865 (12) | 0.0130 (4) |
| H9A | 0.3557 | -0.1085 | 0.2150 | 0.016* |
| H9B | 0.4406 | -0.1030 | 0.2124 | 0.016* |
| C10 | 0.45890 (10) | 0.04737 (15) | 0.10849 (12) | 0.0117 (4) |
| H10A | 0.4525 | 0.0847 | 0.0573 | 0.014* |
| H10B | 0.4672 | 0.0966 | 0.1523 | 0.014* |
| C11 | 0.37745 (11) | -0.09448 (16) | 0.06228 (12) | 0.0131 (4) |
| H11A | 0.4167 | -0.1436 | 0.0668 | 0.016* |
| H11B | 0.3331 | -0.1296 | 0.0762 | 0.016* |
| C12 | 0.23527 (12) | 0.06420 (17) | 0.30964 (14) | 0.0191 (5) |
| H12A | 0.2208 | 0.0044 | 0.2781 | 0.023* |
| H12B | 0.2500 | 0.0410 | 0.3642 | 0.023* |
| C13 | 0.17028 (12) | 0.13118 (19) | 0.31788 (16) | 0.0259 (5) |
| H13A | 0.1816 | 0.1846 | 0.3574 | 0.031* |
| H13B | 0.1597 | 0.1635 | 0.2652 | 0.031* |
| C14 | 0.10488 (13) | 0.07612 (19) | 0.34454 (17) | 0.0272 (5) |
| H14A | 0.1168 | 0.0397 | 0.3951 | 0.033* |
| H14B | 0.0918 | 0.0258 | 0.3030 | 0.033* |
| C15 | 0.04070 (14) | 0.1421 (2) | 0.35880 (18) | 0.0350 (7) |
| H15A | 0.0495 | 0.1833 | 0.4069 | 0.052* |
| H15B | -0.0012 | 0.1001 | 0.3669 | 0.052* |
| H15C | 0.0323 | 0.1854 | 0.3119 | 0.052* |
| C16 | 0.40219 (11) | 0.23185 (17) | 0.30125 (13) | 0.0164 (4) |
| H16A | 0.4161 | 0.2102 | 0.3565 | 0.020* |
| H16B | 0.4451 | 0.2276 | 0.2680 | 0.020* |
| C17 | 0.37945 (12) | 0.34137 (17) | 0.30495 (14) | 0.0180 (5) |
| H17A | 0.4205 | 0.3818 | 0.3243 | 0.022* |
| H17B | 0.3667 | 0.3641 | 0.2496 | 0.022* |
| C18 | 0.31701 (12) | 0.36167 (17) | 0.35918 (14) | 0.0200 (5) |
| H18A | 0.3050 | 0.4336 | 0.3560 | 0.024* |
| H18B | 0.2753 | 0.3237 | 0.3385 | 0.024* |
| C19 | 0.33061 (15) | 0.3340 (2) | 0.44694 (15) | 0.0344 (7) |
| H19A | 0.3368 | 0.2615 | 0.4515 | 0.052* |
| H19B | 0.2901 | 0.3549 | 0.4789 | 0.052* |
| H19C | 0.3737 | 0.3677 | 0.4671 | 0.052* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|-------------|--------------|--------------|
| Sn1 | 0.00935 (7) | 0.01444 (8) | 0.01012 (7) | 0.00111 (5) | -0.00151 (5) | -0.00132 (5) |
| Br1 | 0.01670 (11) | 0.02112 (12) | 0.02432 (12) | 0.00431 (9) | -0.01116 (9) | -0.00292 (9) |
| N1 | 0.0092 (8) | 0.0119 (8) | 0.0140 (8) | 0.0008 (7) | 0.0000 (6) | 0.0013 (7) |
| O1 | 0.0171 (8) | 0.0148 (7) | 0.0139 (7) | 0.0022 (6) | -0.0048 (6) | -0.0024 (6) |
| O2 | 0.0146 (7) | 0.0160 (7) | 0.0116 (7) | 0.0034 (6) | -0.0035 (6) | -0.0013 (6) |
| O3 | 0.0092 (7) | 0.0196 (8) | 0.0127 (7) | 0.0046 (6) | -0.0028 (6) | -0.0026 (6) |
| O4 | 0.0133 (7) | 0.0214 (8) | 0.0107 (7) | -0.0014 (6) | 0.0005 (6) | -0.0005 (6) |
| C1 | 0.0097 (9) | 0.0143 (10) | 0.0117 (10) | 0.0006 (8) | -0.0013 (8) | 0.0013 (8) |
| C2 | 0.0128 (10) | 0.0164 (10) | 0.0105 (9) | -0.0011 (8) | 0.0001 (8) | 0.0010 (8) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C3 | 0.0185 (11) | 0.0149 (10) | 0.0126 (10) | 0.0024 (9) | 0.0015 (8) | -0.0015 (8) |
| C4 | 0.0131 (10) | 0.0190 (11) | 0.0144 (10) | 0.0034 (9) | 0.0003 (8) | 0.0031 (8) |
| C5 | 0.0117 (10) | 0.0188 (11) | 0.0138 (10) | -0.0011 (9) | -0.0042 (8) | 0.0028 (8) |
| C6 | 0.0140 (10) | 0.0154 (10) | 0.0136 (10) | 0.0012 (8) | -0.0023 (8) | -0.0004 (8) |
| C7 | 0.0119 (10) | 0.0128 (10) | 0.0129 (10) | -0.0002 (8) | 0.0018 (8) | 0.0001 (8) |
| C8 | 0.0096 (9) | 0.0127 (10) | 0.0124 (10) | 0.0032 (8) | -0.0003 (7) | 0.0003 (8) |
| C9 | 0.0120 (10) | 0.0141 (10) | 0.0128 (10) | 0.0027 (8) | -0.0009 (8) | 0.0001 (8) |
| C10 | 0.0095 (9) | 0.0140 (10) | 0.0114 (10) | 0.0009 (8) | -0.0010 (7) | -0.0002 (8) |
| C11 | 0.0110 (9) | 0.0144 (10) | 0.0138 (10) | -0.0006 (8) | -0.0008 (8) | -0.0009 (8) |
| C12 | 0.0155 (11) | 0.0192 (11) | 0.0227 (12) | -0.0013 (9) | 0.0043 (9) | -0.0017 (9) |
| C13 | 0.0166 (12) | 0.0316 (14) | 0.0298 (13) | 0.0049 (10) | 0.0043 (10) | 0.0099 (11) |
| C14 | 0.0196 (12) | 0.0264 (13) | 0.0359 (14) | -0.0035 (11) | 0.0077 (10) | -0.0110 (11) |
| C15 | 0.0179 (13) | 0.0498 (18) | 0.0376 (16) | 0.0035 (12) | 0.0062 (11) | 0.0078 (13) |
| C16 | 0.0115 (10) | 0.0193 (11) | 0.0183 (11) | 0.0024 (9) | -0.0016 (8) | -0.0034 (9) |
| C17 | 0.0177 (11) | 0.0174 (11) | 0.0188 (11) | -0.0003 (9) | -0.0035 (9) | -0.0014 (9) |
| C18 | 0.0201 (11) | 0.0197 (11) | 0.0199 (11) | 0.0051 (9) | -0.0042 (9) | -0.0049 (9) |
| C19 | 0.0313 (14) | 0.0536 (18) | 0.0184 (12) | 0.0169 (14) | 0.0004 (11) | 0.0000 (12) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| Sn1—N1 | 2.2108 (17) | C9—H9B | 0.9900 |
| Sn1—O1 | 2.1203 (15) | C10—H10A | 0.9900 |
| Sn1—O2 | 2.1049 (14) | C10—H10B | 0.9900 |
| Sn1—C12 | 2.139 (2) | C11—H11A | 0.9900 |
| Sn1—C16 | 2.129 (2) | C11—H11B | 0.9900 |
| Br1—C5 | 1.901 (2) | C12—C13 | 1.526 (3) |
| N1—C7 | 1.289 (3) | C12—H12A | 0.9900 |
| N1—C8 | 1.487 (3) | C12—H12B | 0.9900 |
| O1—C2 | 1.317 (2) | C13—C14 | 1.510 (3) |
| O2—C9 | 1.405 (2) | C13—H13A | 0.9900 |
| O3—C10 | 1.422 (2) | C13—H13B | 0.9900 |
| O3—H3 | 0.8400 | C14—C15 | 1.520 (3) |
| O4—C11 | 1.418 (2) | C14—H14A | 0.9900 |
| O4—H4 | 0.8400 | C14—H14B | 0.9900 |
| C1—C6 | 1.408 (3) | C15—H15A | 0.9800 |
| C1—C2 | 1.419 (3) | C15—H15B | 0.9800 |
| C1—C7 | 1.445 (3) | C15—H15C | 0.9800 |
| C2—C3 | 1.408 (3) | C16—C17 | 1.528 (3) |
| C3—C4 | 1.379 (3) | C16—H16A | 0.9900 |
| C3—H3A | 0.9500 | C16—H16B | 0.9900 |
| C4—C5 | 1.401 (3) | C17—C18 | 1.522 (3) |
| C4—H4A | 0.9500 | C17—H17A | 0.9900 |
| C5—C6 | 1.368 (3) | C17—H17B | 0.9900 |
| C6—H6 | 0.9500 | C18—C19 | 1.517 (3) |
| C7—H7 | 0.9500 | C18—H18A | 0.9900 |
| C8—C11 | 1.534 (3) | C18—H18B | 0.9900 |
| C8—C10 | 1.535 (3) | C19—H19A | 0.9800 |
| C8—C9 | 1.543 (3) | C19—H19B | 0.9800 |

| | | | |
|-------------|-------------|---------------|-------------|
| C9—H9A | 0.9900 | C19—H19C | 0.9800 |
| O2—Sn1—O1 | 155.60 (6) | H10A—C10—H10B | 108.0 |
| O2—Sn1—C16 | 91.43 (7) | O4—C11—C8 | 116.38 (17) |
| O1—Sn1—C16 | 91.84 (7) | O4—C11—H11A | 108.2 |
| O2—Sn1—C12 | 98.49 (7) | C8—C11—H11A | 108.2 |
| O1—Sn1—C12 | 97.86 (8) | O4—C11—H11B | 108.2 |
| C16—Sn1—C12 | 129.92 (9) | C8—C11—H11B | 108.2 |
| O2—Sn1—N1 | 76.29 (6) | H11A—C11—H11B | 107.3 |
| O1—Sn1—N1 | 81.56 (6) | C13—C12—Sn1 | 116.87 (16) |
| C16—Sn1—N1 | 122.33 (7) | C13—C12—H12A | 108.1 |
| C12—Sn1—N1 | 107.69 (8) | Sn1—C12—H12A | 108.1 |
| C7—N1—C8 | 121.31 (18) | C13—C12—H12B | 108.1 |
| C7—N1—Sn1 | 124.39 (14) | Sn1—C12—H12B | 108.1 |
| C8—N1—Sn1 | 113.83 (12) | H12A—C12—H12B | 107.3 |
| C2—O1—Sn1 | 125.58 (13) | C14—C13—C12 | 113.7 (2) |
| C9—O2—Sn1 | 115.39 (12) | C14—C13—H13A | 108.8 |
| C10—O3—H3 | 109.5 | C12—C13—H13A | 108.8 |
| C11—O4—H4 | 109.5 | C14—C13—H13B | 108.8 |
| C6—C1—C2 | 120.06 (19) | C12—C13—H13B | 108.8 |
| C6—C1—C7 | 116.66 (19) | H13A—C13—H13B | 107.7 |
| C2—C1—C7 | 123.25 (19) | C13—C14—C15 | 114.8 (2) |
| O1—C2—C3 | 119.74 (19) | C13—C14—H14A | 108.6 |
| O1—C2—C1 | 122.45 (19) | C15—C14—H14A | 108.6 |
| C3—C2—C1 | 117.81 (19) | C13—C14—H14B | 108.6 |
| C4—C3—C2 | 121.5 (2) | C15—C14—H14B | 108.6 |
| C4—C3—H3A | 119.2 | H14A—C14—H14B | 107.5 |
| C2—C3—H3A | 119.2 | C14—C15—H15A | 109.5 |
| C3—C4—C5 | 119.6 (2) | C14—C15—H15B | 109.5 |
| C3—C4—H4A | 120.2 | H15A—C15—H15B | 109.5 |
| C5—C4—H4A | 120.2 | C14—C15—H15C | 109.5 |
| C6—C5—C4 | 120.8 (2) | H15A—C15—H15C | 109.5 |
| C6—C5—Br1 | 120.16 (16) | H15B—C15—H15C | 109.5 |
| C4—C5—Br1 | 119.09 (16) | C17—C16—Sn1 | 116.73 (14) |
| C5—C6—C1 | 120.2 (2) | C17—C16—H16A | 108.1 |
| C5—C6—H6 | 119.9 | Sn1—C16—H16A | 108.1 |
| C1—C6—H6 | 119.9 | C17—C16—H16B | 108.1 |
| N1—C7—C1 | 126.66 (19) | Sn1—C16—H16B | 108.1 |
| N1—C7—H7 | 116.7 | H16A—C16—H16B | 107.3 |
| C1—C7—H7 | 116.7 | C18—C17—C16 | 114.59 (19) |
| N1—C8—C11 | 115.35 (16) | C18—C17—H17A | 108.6 |
| N1—C8—C10 | 105.98 (16) | C16—C17—H17A | 108.6 |
| C11—C8—C10 | 112.19 (16) | C18—C17—H17B | 108.6 |
| N1—C8—C9 | 104.99 (15) | C16—C17—H17B | 108.6 |
| C11—C8—C9 | 107.46 (17) | H17A—C17—H17B | 107.6 |
| C10—C8—C9 | 110.64 (16) | C19—C18—C17 | 114.1 (2) |
| O2—C9—C8 | 111.04 (17) | C19—C18—H18A | 108.7 |
| O2—C9—H9A | 109.4 | C17—C18—H18A | 108.7 |

| | | | |
|---------------|--------------|-----------------|--------------|
| C8—C9—H9A | 109.4 | C19—C18—H18B | 108.7 |
| O2—C9—H9B | 109.4 | C17—C18—H18B | 108.7 |
| C8—C9—H9B | 109.4 | H18A—C18—H18B | 107.6 |
| H9A—C9—H9B | 108.0 | C18—C19—H19A | 109.5 |
| O3—C10—C8 | 111.57 (16) | C18—C19—H19B | 109.5 |
| O3—C10—H10A | 109.3 | H19A—C19—H19B | 109.5 |
| C8—C10—H10A | 109.3 | C18—C19—H19C | 109.5 |
| O3—C10—H10B | 109.3 | H19A—C19—H19C | 109.5 |
| C8—C10—H10B | 109.3 | H19B—C19—H19C | 109.5 |
| | | | |
| O2—Sn1—N1—C7 | 161.51 (18) | Sn1—N1—C7—C1 | 8.4 (3) |
| O1—Sn1—N1—C7 | -28.79 (17) | C6—C1—C7—N1 | -166.4 (2) |
| C16—Sn1—N1—C7 | -115.61 (17) | C2—C1—C7—N1 | 15.8 (3) |
| C12—Sn1—N1—C7 | 66.82 (18) | C7—N1—C8—C11 | -22.0 (3) |
| O2—Sn1—N1—C8 | -10.66 (12) | Sn1—N1—C8—C11 | 150.45 (14) |
| O1—Sn1—N1—C8 | 159.04 (14) | C7—N1—C8—C10 | 102.8 (2) |
| C16—Sn1—N1—C8 | 72.22 (15) | Sn1—N1—C8—C10 | -84.77 (15) |
| C12—Sn1—N1—C8 | -105.35 (14) | C7—N1—C8—C9 | -140.06 (19) |
| O2—Sn1—O1—C2 | 67.9 (2) | Sn1—N1—C8—C9 | 32.38 (18) |
| C16—Sn1—O1—C2 | 165.50 (16) | Sn1—O2—C9—C8 | 41.10 (19) |
| C12—Sn1—O1—C2 | -63.76 (17) | N1—C8—C9—O2 | -46.7 (2) |
| N1—Sn1—O1—C2 | 43.07 (16) | C11—C8—C9—O2 | -169.96 (16) |
| O1—Sn1—O2—C9 | -42.4 (2) | C10—C8—C9—O2 | 67.3 (2) |
| C16—Sn1—O2—C9 | -140.00 (14) | N1—C8—C10—O3 | 177.90 (15) |
| C12—Sn1—O2—C9 | 89.25 (14) | C11—C8—C10—O3 | -55.4 (2) |
| N1—Sn1—O2—C9 | -17.01 (13) | C9—C8—C10—O3 | 64.6 (2) |
| Sn1—O1—C2—C3 | 144.75 (16) | N1—C8—C11—O4 | 63.8 (2) |
| Sn1—O1—C2—C1 | -36.3 (3) | C10—C8—C11—O4 | -57.7 (2) |
| C6—C1—C2—O1 | -179.37 (19) | C9—C8—C11—O4 | -179.53 (16) |
| C7—C1—C2—O1 | -1.7 (3) | O2—Sn1—C12—C13 | 174.84 (17) |
| C6—C1—C2—C3 | -0.4 (3) | O1—Sn1—C12—C13 | -23.33 (19) |
| C7—C1—C2—C3 | 177.28 (19) | C16—Sn1—C12—C13 | 75.8 (2) |
| O1—C2—C3—C4 | -177.65 (19) | N1—Sn1—C12—C13 | -106.93 (18) |
| C1—C2—C3—C4 | 3.4 (3) | Sn1—C12—C13—C14 | 170.31 (17) |
| C2—C3—C4—C5 | -2.9 (3) | C12—C13—C14—C15 | 176.0 (2) |
| C3—C4—C5—C6 | -0.7 (3) | O2—Sn1—C16—C17 | -179.92 (16) |
| C3—C4—C5—Br1 | 179.46 (16) | O1—Sn1—C16—C17 | 24.26 (16) |
| C4—C5—C6—C1 | 3.6 (3) | C12—Sn1—C16—C17 | -77.59 (19) |
| Br1—C5—C6—C1 | -176.54 (16) | N1—Sn1—C16—C17 | 105.44 (16) |
| C2—C1—C6—C5 | -3.0 (3) | Sn1—C16—C17—C18 | 62.2 (2) |
| C7—C1—C6—C5 | 179.12 (19) | C16—C17—C18—C19 | 60.7 (3) |
| C8—N1—C7—C1 | 179.97 (19) | | |

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—H3...O2 ⁱ | 0.84 | 1.77 | 2.608 (2) | 174 |

| | | | | |
|--------------------------|------|------|-----------|-----|
| O4—H4···O3 ⁱⁱ | 0.84 | 1.93 | 2.733 (2) | 160 |
|--------------------------|------|------|-----------|-----|

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