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# Dichlorido{1-[N-(5-chloro-2-oxo-phenyl)carboximidoyl]naphthalen-2-olato- $\kappa^3 O,N,O'$ }(methanol- $\kappa O$ )tin(IV)

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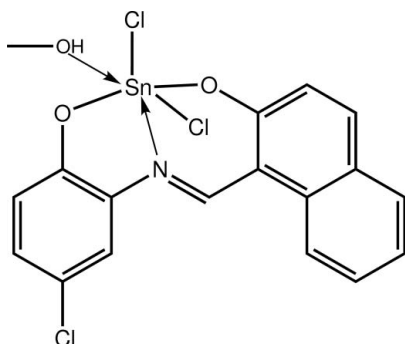
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.059; data-to-parameter ratio = 17.3.

In the title complex,  $[Sn(C_{17}H_{10}ClNO_2)Cl_2(CH_3OH)]$ , the  $Sn^{IV}$  atom features a distorted octahedral geometry defined by the  $O,N,O'$ -donors of the dianion, two Cl atoms and the methanol O atom. The six-membered chelate ring has a half-chair conformation with the Sn atom lying 0.449 (4) Å out of the plane defined by the remaining atoms (r.m.s. deviation = 0.0238 Å). Supramolecular helical chains along [100], mediated by  $O-H \cdots O$  hydrogen bonds, feature in the crystal packing. Chains are linked by  $C-H \cdots O$ ,  $C-H \cdots Cl$  and  $\pi-\pi$  [centroid-centroid distance = 3.598 (2) Å] interactions.

## Related literature

For background to related Sn(IV) Schiff base compounds and a closely related structure, see: Pettinari *et al.* (2001). For specialized crystallization techniques, see: Harrowfield *et al.* (1996).



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## Experimental

### Crystal data

$[Sn(C_{17}H_{10}ClNO_2)Cl_2(CH_3O)]$   
 $M_r = 517.34$   
Orthorhombic,  $P2_12_12_1$   
 $a = 9.9767$  (3) Å  
 $b = 11.1639$  (3) Å  
 $c = 16.2755$  (5) Å  
 $V = 1812.75$  (9) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 1.87$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.25 \times 0.20 \times 0.15$  mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector  
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)  
 $T_{min} = 0.819$ ,  $T_{max} = 1.000$   
6571 measured reflections  
4139 independent reflections  
3913 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.024$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.059$   
 $S = 1.01$   
4139 reflections  
239 parameters  
1 restraint  
H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 0.54$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.73$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983), 1765 Friedel pairs  
Flack parameter:  $-0.036$  (19)

**Table 1**

Selected bond lengths (Å).

Sn—Cl1	2.3398 (10)	Sn—O2	2.010 (3)
Sn—Cl2	2.3807 (9)	Sn—O3	2.174 (3)
Sn—O1	2.050 (2)	Sn—N1	2.144 (3)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O3-H3O \cdots O1^i$	0.84 (1)	1.80 (1)	2.633 (4)	174 (4)
$C2-H2 \cdots O2^{ii}$	0.95	2.50	3.363 (4)	151
$C16-H16 \cdots Cl3^{iii}$	0.95	2.74	3.542 (4)	143
$C18-H18A \cdots Cl2^i$	0.98	2.77	3.707 (4)	161

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We gratefully acknowledge support of this study by Tabriz Azad University, and thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5171).

## References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.

- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst. A* **39**, 876–881.
- Harrowfield, J. M., Miyamae, H., Skelton, B. W., Soudi, A. A. & White, A. H. (1996). *Aust. J. Chem.* **49**, 1165–1169.
- Pettinari, C., Marchetti, F., Pettinari, R., Martini, D., Drozdov, A. & Troyanov, S. (2001). *Inorg. Chim. Acta*, **325**, 103–114.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## supporting information

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## Dichlorido{1-[*N*-(5-chloro-2-oxidophenyl)carboximidoyl]naphthalen-2-olato- $\kappa^3O,N,O$ }(methanol- $\kappa O$ )tin(IV)

Gholam Hossein Shahverdizadeh, Seik Weng Ng, Edward R. T. Tiekink and Babak Mirtamizdoust

### S1. Comment

Original interest in tin(IV) compounds with Schiff bases ligands based on the 2-[(2-hydroxyphenyl)imino]methyl}-phenol parent compound stemmed from possible applications in medicinal chemistry (Pettinari *et al.*, 2001). This motivated the synthesis and characterization of the title compound, (I).

In (I), Fig. 1, the Sn<sup>IV</sup> atom is coordinated by the tridentate, dinegative Schiff base, two Cl atoms and the O atom of a methanol molecule to define a distorted octahedral geometry within a Cl<sub>2</sub>NO<sub>3</sub> donor set, Table 1. The five-membered chelate ring is approximately planar with a r.m.s. deviation of 0.058 Å. By contrast, the six-membered chelate ring has a half-chair conformation as the Sn atom lies 0.449 (4) Å out of the plane defined by the five remaining atoms (r.m.s. deviation = 0.024 Å). The Sn—Cl2 bond length is significantly longer than that of Sn—Cl1, a difference which is correlated with the Cl2 atom being *trans* to the methanol-*O* atom.

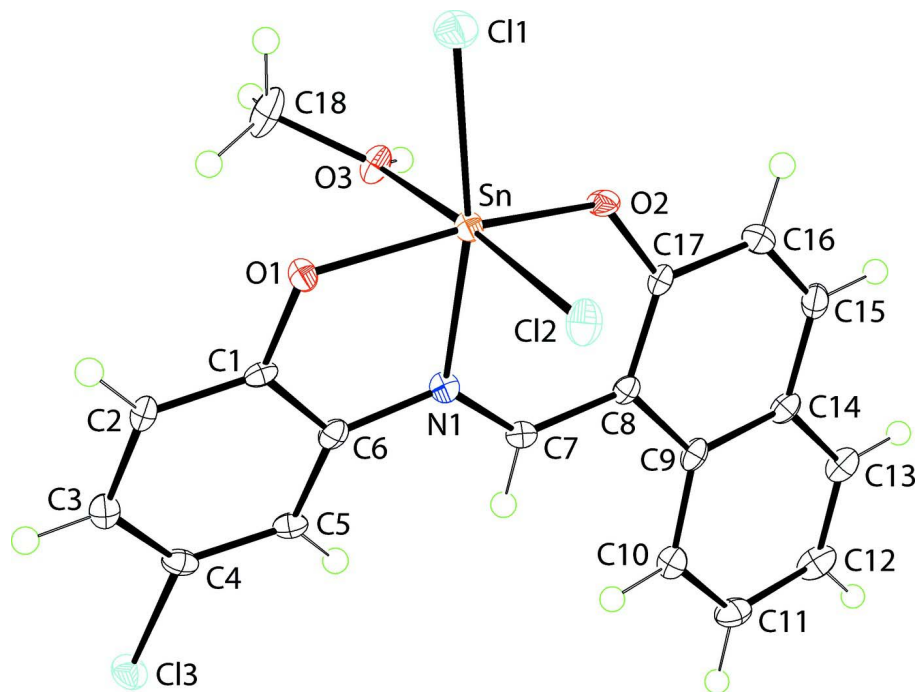
The most significant feature of the crystal packing is the formation of helical supramolecular chains along [100] mediated by O—H $\cdots$ O hydrogen bonding, Fig. 2 and Table 2. Chains are consolidated in the crystal packing by C—H $\cdots$ O and C—H $\cdots$ Cl interactions. Further stability is provided by  $\pi$ – $\pi$  contacts [ring centroid(C1–C6) $\cdots$ ring centroid(C8,C9,C14–C17)]<sup>*i*</sup> = 3.598 (2) Å, angle = 10.47 (17)° for *i*: 1 - *x*, 1/2 + *y*, 3/2 - *z*).

### S2. Experimental

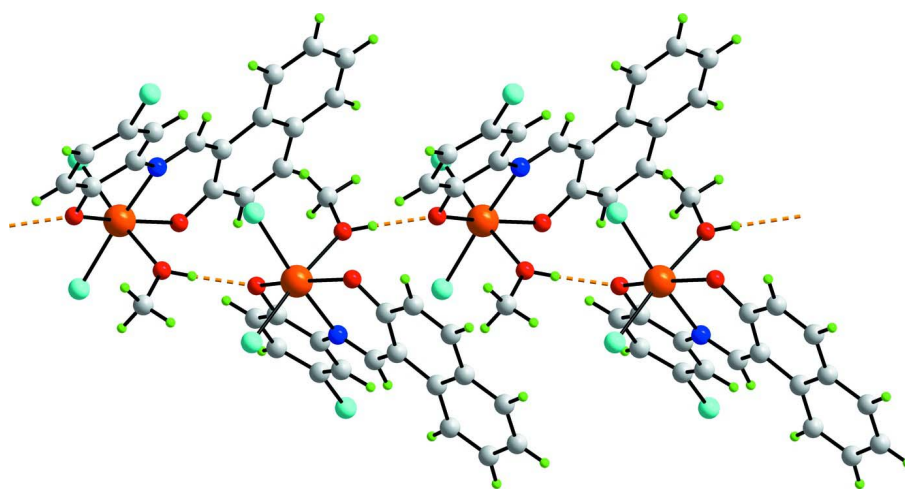
A solution of 2-amino-4-chlorophenol (10 mmol) in EtOH (30 ml) was added drop-wise to the solution of 2-hydroxy-1-naphthaldehyde (10 mmol) in EtOH (20 ml). The mixture was refluxed for 5 h. The yellow precipitate was removed by filtration and recrystallized from MeOH solution. The ligand (0.5 mmol) was placed in one arm of a branched tube (Harrowfield *et al.*, 1996) and tin(IV) chloride (0.5 mmol) in the other. Methanol was then added to fill both arms, the tube sealed and the ligand-containing arm immersed in a bath at 333 K, while the other was left at ambient temperature. After three weeks crystals deposited in the arm held at ambient temperature. They were filtered off, washed with acetone and ether, and air-dried. Yield: 68%. *M.pt.*: 571 K (dec.).

### S3. Refinement

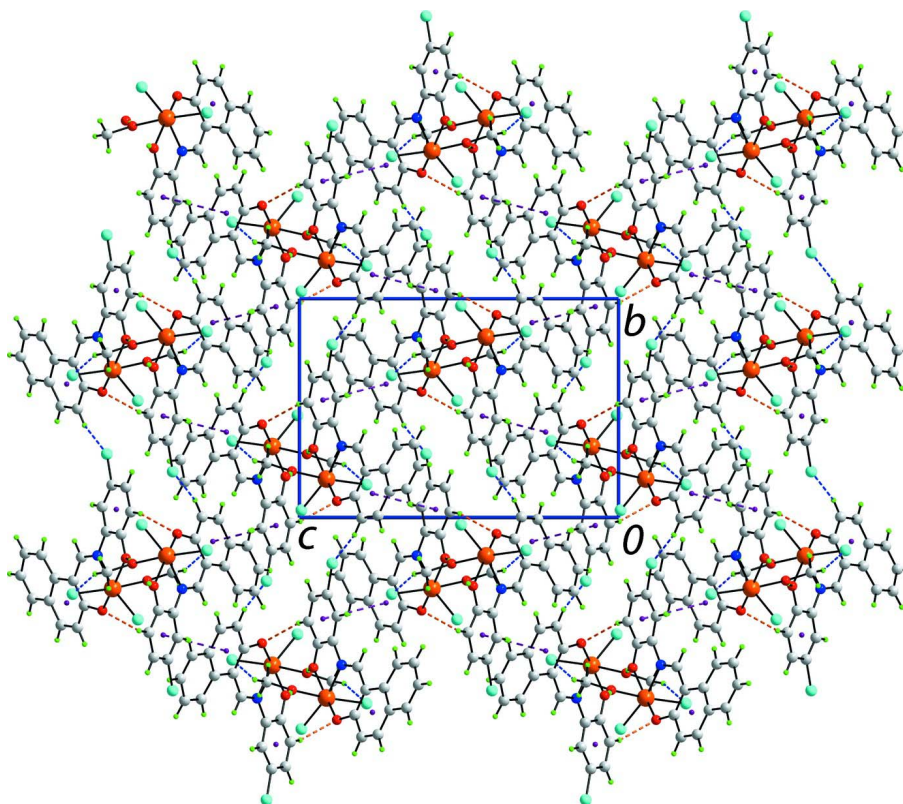
Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.98 Å and with  $U_{\text{iso}}(\text{H}) = 1.2$  to  $1.5U_{\text{eq}}(\text{C})$ ] and were included in the refinement in the riding model approximation. The hydroxy H-atom was located in a difference Fourier map and was refined with a distance restraint of O—H = 0.84±0.01 Å;  $U_{\text{iso}}$  was refined. The (0 1 1) reflection was omitted from the final refinement owing to poor agreement.

**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

**Figure 2**

View of the supramolecular chain along [100] in (I) mediated by O—H...O hydrogen bonding shown as orange dashed lines.

**Figure 3**

A view in projection down the  $a$  axis of the unit-cell contents of (I). The C—H...O, C—H...Cl and  $\pi$ - $\pi$  interactions are shown as orange, blue and purple dashed lines.

### Dichlorido[1-[N-(5-chloro-2-oxidophenyl)carboximidoyl]naphthalen-2-olato- $\kappa^3O,N,O'$ ](methanol- $\kappa O$ )tin(IV)

#### Crystal data

[Sn(C<sub>17</sub>H<sub>10</sub>ClNO<sub>2</sub>)Cl<sub>2</sub>(CH<sub>4</sub>O)]

$M_r = 517.34$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 9.9767$  (3) Å

$b = 11.1639$  (3) Å

$c = 16.2755$  (5) Å

$V = 1812.75$  (9) Å<sup>3</sup>

$Z = 4$

$F(000) = 1016$

$D_x = 1.896$  Mg m<sup>-3</sup>

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

Cell parameters from 4166 reflections

$\theta = 2.2$ – $27.5^\circ$

$\mu = 1.87$  mm<sup>-1</sup>

$T = 100$  K

Prism, brown

$0.25 \times 0.20 \times 0.15$  mm

#### Data collection

Agilent SuperNova Dual

diffractometer with an Atlas detector

Radiation source: SuperNova (Mo) X-ray

Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  scan

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.819$ ,  $T_{\max} = 1.000$

6571 measured reflections

4139 independent reflections

3913 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.6^\circ$ ,  $\theta_{\min} = 2.4^\circ$

$h = -12 \rightarrow 7$

$k = -10 \rightarrow 14$

$l = -21 \rightarrow 20$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.059$   
 $S = 1.01$   
 4139 reflections  
 239 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0231P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: Flack (1983), 1765 Friedel  
 pairs  
 Absolute structure parameter:  $-0.036$  (19)

Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn	0.39500 (3)	0.17557 (2)	0.915201 (14)	0.01147 (6)
Cl1	0.27998 (11)	0.03339 (8)	0.99384 (6)	0.0222 (2)
Cl2	0.27645 (10)	0.15018 (8)	0.78945 (5)	0.0197 (2)
Cl3	0.50466 (11)	0.79039 (7)	0.89690 (6)	0.0188 (2)
O1	0.2770 (2)	0.3133 (2)	0.95636 (14)	0.0121 (5)
O2	0.5532 (3)	0.0747 (2)	0.88264 (15)	0.0146 (6)
O3	0.5167 (3)	0.2113 (2)	1.02329 (15)	0.0149 (6)
H3O	0.5989 (13)	0.198 (3)	1.029 (2)	0.021 (11)*
N1	0.5035 (3)	0.3262 (3)	0.86761 (16)	0.0119 (6)
C1	0.3288 (4)	0.4240 (3)	0.9413 (2)	0.0113 (8)
C2	0.2641 (4)	0.5253 (3)	0.9715 (2)	0.0112 (7)
H2	0.1836	0.5175	1.0023	0.013*
C3	0.3185 (4)	0.6384 (3)	0.9563 (2)	0.0137 (8)
H3	0.2741	0.7083	0.9756	0.016*
C4	0.4377 (4)	0.6482 (3)	0.9128 (2)	0.0136 (7)
C5	0.5029 (4)	0.5491 (3)	0.8821 (2)	0.0124 (8)
H5	0.5840	0.5580	0.8521	0.015*
C6	0.4490 (4)	0.4361 (3)	0.8953 (2)	0.0123 (8)
C7	0.6067 (4)	0.3186 (3)	0.81737 (18)	0.0125 (7)
H7	0.6401	0.3918	0.7958	0.015*
C8	0.6736 (4)	0.2118 (3)	0.7921 (2)	0.0110 (7)
C9	0.7848 (4)	0.2219 (3)	0.7340 (2)	0.0133 (8)
C10	0.8181 (4)	0.3302 (4)	0.6923 (2)	0.0144 (7)

H10	0.7644	0.3995	0.7006	0.017*
C11	0.9261 (4)	0.3361 (3)	0.6407 (2)	0.0189 (8)
H11	0.9456	0.4093	0.6135	0.023*
C12	1.0089 (4)	0.2361 (3)	0.6272 (2)	0.0196 (9)
H12	1.0856	0.2423	0.5929	0.023*
C13	0.9775 (4)	0.1303 (3)	0.6639 (2)	0.0166 (8)
H13	1.0317	0.0619	0.6538	0.020*
C14	0.8661 (4)	0.1203 (3)	0.7168 (2)	0.0138 (8)
C15	0.8323 (4)	0.0086 (3)	0.7535 (2)	0.0172 (8)
H15	0.8852	-0.0599	0.7413	0.021*
C16	0.7278 (4)	-0.0026 (3)	0.8048 (2)	0.0175 (9)
H16	0.7070	-0.0790	0.8271	0.021*
C17	0.6474 (4)	0.0978 (3)	0.8264 (2)	0.0115 (8)
C18	0.4697 (4)	0.2485 (4)	1.1025 (2)	0.0243 (10)
H18A	0.5462	0.2583	1.1397	0.036*
H18B	0.4087	0.1877	1.1247	0.036*
H18C	0.4220	0.3249	1.0974	0.036*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn	0.00915 (11)	0.01150 (10)	0.01375 (11)	-0.00087 (11)	0.00154 (11)	-0.00057 (11)
Cl1	0.0196 (5)	0.0204 (4)	0.0265 (5)	-0.0049 (4)	0.0050 (5)	0.0019 (4)
Cl2	0.0179 (5)	0.0225 (5)	0.0187 (4)	-0.0008 (4)	-0.0027 (4)	-0.0060 (4)
Cl3	0.0204 (5)	0.0125 (4)	0.0237 (5)	-0.0033 (4)	0.0017 (4)	-0.0002 (3)
O1	0.0082 (13)	0.0103 (11)	0.0176 (12)	-0.0012 (11)	0.0042 (10)	-0.0011 (11)
O2	0.0136 (15)	0.0138 (12)	0.0166 (12)	0.0019 (10)	0.0064 (11)	0.0044 (11)
O3	0.0062 (14)	0.0246 (14)	0.0138 (12)	0.0026 (12)	0.0009 (12)	-0.0019 (11)
N1	0.0089 (15)	0.0126 (13)	0.0141 (13)	-0.0011 (15)	-0.0002 (12)	-0.0006 (14)
C1	0.012 (2)	0.0145 (16)	0.0078 (15)	-0.0021 (15)	-0.0013 (15)	0.0028 (14)
C2	0.0077 (19)	0.0168 (16)	0.0091 (16)	0.0018 (15)	-0.0013 (15)	-0.0028 (15)
C3	0.012 (2)	0.0154 (17)	0.0135 (17)	0.0014 (15)	-0.0021 (16)	-0.0020 (15)
C4	0.0153 (19)	0.0120 (16)	0.0137 (15)	-0.0025 (13)	-0.0055 (16)	0.0029 (16)
C5	0.010 (2)	0.0152 (17)	0.0124 (16)	-0.0014 (15)	-0.0013 (16)	0.0041 (15)
C6	0.0124 (19)	0.0162 (16)	0.0082 (17)	0.0005 (14)	-0.0024 (14)	-0.0002 (14)
C7	0.0123 (17)	0.0130 (14)	0.0122 (15)	-0.0007 (19)	-0.0006 (15)	0.0019 (15)
C8	0.0089 (19)	0.0152 (17)	0.0088 (16)	0.0019 (14)	-0.0014 (14)	0.0000 (14)
C9	0.011 (2)	0.0194 (17)	0.0096 (16)	-0.0009 (16)	-0.0011 (16)	-0.0028 (15)
C10	0.0099 (18)	0.0185 (17)	0.0148 (16)	0.0017 (17)	-0.0004 (14)	-0.0010 (17)
C11	0.019 (2)	0.0210 (18)	0.0165 (16)	-0.0055 (18)	0.0011 (15)	0.0042 (17)
C12	0.009 (2)	0.033 (2)	0.0164 (19)	-0.0003 (18)	0.0017 (17)	0.0039 (18)
C13	0.009 (2)	0.0265 (19)	0.0142 (17)	0.0038 (16)	0.0000 (16)	0.0002 (17)
C14	0.009 (2)	0.0210 (18)	0.0110 (16)	-0.0010 (15)	0.0012 (15)	-0.0001 (15)
C15	0.020 (2)	0.0184 (19)	0.0131 (18)	0.0062 (16)	-0.0024 (17)	-0.0034 (16)
C16	0.021 (2)	0.0137 (17)	0.0176 (18)	0.0028 (17)	0.0003 (17)	0.0024 (16)
C17	0.0099 (19)	0.0155 (16)	0.0089 (16)	0.0004 (15)	-0.0001 (14)	-0.0021 (15)
C18	0.016 (2)	0.043 (2)	0.0141 (19)	0.0063 (19)	0.0019 (17)	-0.0063 (18)

*Geometric parameters (Å, °)*

Sn—C11	2.3398 (10)	C7—C8	1.427 (5)
Sn—C12	2.3807 (9)	C7—H7	0.9500
Sn—O1	2.050 (2)	C8—C17	1.414 (5)
Sn—O2	2.010 (3)	C8—C9	1.462 (5)
Sn—O3	2.174 (3)	C9—C14	1.422 (5)
Sn—N1	2.144 (3)	C9—C10	1.426 (5)
C13—C4	1.742 (3)	C10—C11	1.368 (5)
O1—C1	1.361 (4)	C10—H10	0.9500
O2—C17	1.337 (4)	C11—C12	1.406 (5)
O3—C18	1.434 (4)	C11—H11	0.9500
O3—H3O	0.840 (10)	C12—C13	1.360 (5)
N1—C7	1.318 (4)	C12—H12	0.9500
N1—C6	1.416 (5)	C13—C14	1.410 (5)
C1—C2	1.392 (5)	C13—H13	0.9500
C1—C6	1.420 (5)	C14—C15	1.423 (5)
C2—C3	1.397 (5)	C15—C16	1.342 (5)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.388 (5)	C16—C17	1.422 (5)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.377 (5)	C18—H18A	0.9800
C5—C6	1.388 (5)	C18—H18B	0.9800
C5—H5	0.9500	C18—H18C	0.9800
O2—Sn—O1	163.28 (10)	N1—C6—C1	114.2 (3)
O2—Sn—N1	87.01 (11)	N1—C7—C8	126.7 (3)
O1—Sn—N1	79.61 (11)	N1—C7—H7	116.6
O2—Sn—O3	82.99 (10)	C8—C7—H7	116.6
O1—Sn—O3	85.31 (10)	C17—C8—C7	123.5 (3)
N1—Sn—O3	82.33 (10)	C17—C8—C9	117.7 (3)
O2—Sn—C11	98.58 (7)	C7—C8—C9	118.5 (3)
O1—Sn—C11	92.78 (7)	C14—C9—C10	116.7 (3)
N1—Sn—C11	167.70 (8)	C14—C9—C8	119.9 (3)
O3—Sn—C11	87.47 (7)	C10—C9—C8	123.3 (3)
O2—Sn—C12	95.55 (8)	C11—C10—C9	121.0 (4)
O1—Sn—C12	94.87 (7)	C11—C10—H10	119.5
N1—Sn—C12	91.92 (8)	C9—C10—H10	119.5
O3—Sn—C12	174.12 (7)	C10—C11—C12	121.4 (4)
C11—Sn—C12	98.39 (4)	C10—C11—H11	119.3
C1—O1—Sn	113.8 (2)	C12—C11—H11	119.3
C17—O2—Sn	128.6 (2)	C13—C12—C11	119.0 (4)
C18—O3—Sn	126.8 (2)	C13—C12—H12	120.5
C18—O3—H3O	106 (3)	C11—C12—H12	120.5
Sn—O3—H3O	127 (3)	C12—C13—C14	121.2 (4)
C7—N1—C6	123.6 (3)	C12—C13—H13	119.4
C7—N1—Sn	124.6 (3)	C14—C13—H13	119.4
C6—N1—Sn	111.8 (2)	C13—C14—C9	120.4 (3)



O1—C1—C2	119.8 (3)	C13—C14—C15	120.8 (3)
O1—C1—C6	120.1 (3)	C9—C14—C15	118.7 (3)
C2—C1—C6	120.1 (3)	C16—C15—C14	121.8 (4)
C1—C2—C3	119.4 (3)	C16—C15—H15	119.1
C1—C2—H2	120.3	C14—C15—H15	119.1
C3—C2—H2	120.3	C15—C16—C17	121.2 (3)
C4—C3—C2	119.6 (3)	C15—C16—H16	119.4
C4—C3—H3	120.2	C17—C16—H16	119.4
C2—C3—H3	120.2	O2—C17—C8	125.0 (3)
C5—C4—C3	121.8 (3)	O2—C17—C16	114.4 (3)
C5—C4—Cl3	119.8 (3)	C8—C17—C16	120.5 (3)
C3—C4—Cl3	118.4 (3)	O3—C18—H18A	109.5
C4—C5—C6	119.4 (4)	O3—C18—H18B	109.5
C4—C5—H5	120.3	H18A—C18—H18B	109.5
C6—C5—H5	120.3	O3—C18—H18C	109.5
C5—C6—N1	126.2 (3)	H18A—C18—H18C	109.5
C5—C6—C1	119.7 (3)	H18B—C18—H18C	109.5
O2—Sn—O1—C1	31.6 (5)	Sn—N1—C6—C5	173.6 (3)
N1—Sn—O1—C1	-5.7 (2)	C7—N1—C6—C1	173.1 (3)
O3—Sn—O1—C1	77.3 (2)	Sn—N1—C6—C1	-5.7 (4)
Cl1—Sn—O1—C1	164.5 (2)	O1—C1—C6—C5	-178.4 (3)
Cl2—Sn—O1—C1	-96.8 (2)	C2—C1—C6—C5	1.3 (5)
O1—Sn—O2—C17	-59.1 (5)	O1—C1—C6—N1	1.0 (5)
N1—Sn—O2—C17	-22.5 (3)	C2—C1—C6—N1	-179.4 (3)
O3—Sn—O2—C17	-105.1 (3)	C6—N1—C7—C8	174.6 (3)
Cl1—Sn—O2—C17	168.6 (3)	Sn—N1—C7—C8	-6.8 (5)
Cl2—Sn—O2—C17	69.2 (3)	N1—C7—C8—C17	-8.3 (6)
O2—Sn—O3—C18	-156.5 (3)	N1—C7—C8—C9	178.5 (3)
O1—Sn—O3—C18	35.5 (3)	C17—C8—C9—C14	-2.9 (5)
N1—Sn—O3—C18	115.6 (3)	C7—C8—C9—C14	170.7 (3)
Cl1—Sn—O3—C18	-57.5 (3)	C17—C8—C9—C10	177.2 (3)
Cl2—Sn—O3—C18	127.5 (7)	C7—C8—C9—C10	-9.1 (5)
O2—Sn—N1—C7	17.5 (3)	C14—C9—C10—C11	-2.2 (5)
O1—Sn—N1—C7	-172.6 (3)	C8—C9—C10—C11	177.7 (3)
O3—Sn—N1—C7	100.8 (3)	C9—C10—C11—C12	-0.5 (5)
Cl1—Sn—N1—C7	135.0 (3)	C10—C11—C12—C13	2.5 (6)
Cl2—Sn—N1—C7	-78.0 (3)	C11—C12—C13—C14	-1.7 (6)
O2—Sn—N1—C6	-163.7 (2)	C12—C13—C14—C9	-1.0 (6)
O1—Sn—N1—C6	6.2 (2)	C12—C13—C14—C15	178.5 (4)
O3—Sn—N1—C6	-80.4 (2)	C10—C9—C14—C13	2.9 (5)
Cl1—Sn—N1—C6	-46.2 (5)	C8—C9—C14—C13	-176.9 (3)
Cl2—Sn—N1—C6	100.8 (2)	C10—C9—C14—C15	-176.7 (3)
Sn—O1—C1—C2	-175.1 (3)	C8—C9—C14—C15	3.5 (5)
Sn—O1—C1—C6	4.6 (4)	C13—C14—C15—C16	179.1 (4)
O1—C1—C2—C3	179.6 (3)	C9—C14—C15—C16	-1.3 (6)
C6—C1—C2—C3	-0.1 (5)	C14—C15—C16—C17	-1.5 (6)
C1—C2—C3—C4	-1.4 (5)	Sn—O2—C17—C8	16.4 (5)

C2—C3—C4—C5	1.7 (5)	Sn—O2—C17—C16	-166.4 (2)
C2—C3—C4—C13	-178.6 (3)	C7—C8—C17—O2	3.9 (6)
C3—C4—C5—C6	-0.5 (5)	C9—C8—C17—O2	177.3 (3)
C13—C4—C5—C6	179.8 (3)	C7—C8—C17—C16	-173.1 (3)
C4—C5—C6—N1	179.8 (3)	C9—C8—C17—C16	0.2 (5)
C4—C5—C6—C1	-1.0 (5)	C15—C16—C17—O2	-175.3 (3)
C7—N1—C6—C5	-7.6 (5)	C15—C16—C17—C8	2.0 (6)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O3—H3O...O1 <sup>i</sup>	0.84 (1)	1.80 (1)	2.633 (4)	174 (4)
C2—H2...O2 <sup>ii</sup>	0.95	2.50	3.363 (4)	151
C16—H16...C13 <sup>iii</sup>	0.95	2.74	3.542 (4)	143
C18—H18A...C12 <sup>i</sup>	0.98	2.77	3.707 (4)	161

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