

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

[N'-(5-Bromo-2-oxidobenzylidene- κ O)-3-hydroxy-2-naphthohydrazidato- κ^2 N',O]-dicyclohexyltin(IV)

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

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

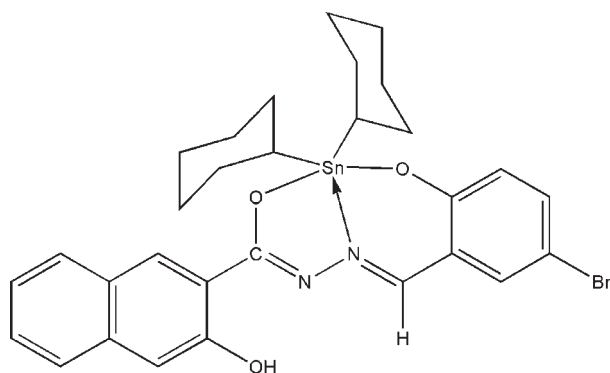
Received 19 November 2009; accepted 9 January 2010

Key indicators: single-crystal X-ray study; $T = 140$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å;
R factor = 0.035; wR factor = 0.079; data-to-parameter ratio = 14.3.

The environment at the Sn^{IV} atom in the title compound, [Sn(C₆H₁₁)₂(C₁₈H₁₁BrN₂O₃)], is distorted trigonal-bipyramidal, with the two cyclohexyl groups and the imino N atom forming the equatorial plane. The axial O—Sn—O angle is 155.97 (9)°. The presence of an intramolecular O—H...N hydrogen bond in the Schiff base ligand helps to stabilize the overall structure.

Related literature

For related structures, see Lee *et al.* (2009a,b). For related dianions of similar hydrazone O,N,O'-chelates to tin in organotin compounds, see: Labib *et al.* (1996); Samanta *et al.* (2007).



Experimental

Crystal data

[Sn(C₆H₁₁)₂(C₁₈H₁₁BrN₂O₃)]
 $M_r = 668.18$
 Monoclinic, $P2_1/c$
 $a = 9.2442$ (2) Å
 $b = 9.9949$ (2) Å
 $c = 29.6493$ (5) Å
 $\beta = 94.874$ (1)°

$V = 2729.54$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.43$ mm⁻¹
 $T = 140$ K
 $0.33 \times 0.30 \times 0.14$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.501$, $T_{\max} = 0.727$

20482 measured reflections
 4787 independent reflections
 4103 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.079$
 $S = 1.09$
 4787 reflections
 335 parameters

1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.60$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3...N2	0.84	1.86	2.600 (4)	146

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 (grant Nos. PS320/2008 C and RG020/09AFR) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2600).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
 Bruker (2008). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Labib, L., Khalil, T. E., Iskander, M. F. & Refaat, L. S. (1996). *Polyhedron*, **21**, 3697–3707.
 Lee, S. M., Lo, K. M., Ali, H. M. & Ng, S. W. (2009b). *Acta Cryst.* **E65**, m862.
 Lee, S. M., Lo, K. M., Mohd Ali, H. & Ng, S. W. (2009a). *Acta Cryst.* **E65**, m816.
 Samanta, B., Chakraborty, J., Dey, D. K. & Mitra, S. (2007). *Struct. Chem.* **18**, 287–297.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Westrip, S. P. (2010). publCIF. In preparation.

supplementary materials

Acta Cryst. (2010). E66, m162 [doi:10.1107/S1600536810001145]

[*N'*-(5-Bromo-2-oxidobenzylidene- κ O)-3-hydroxy-2-naphthohydrazidato- κ^2 *N',O*]dicyclohexyltin(IV)

S. M. Lee, H. Mohd Ali and K. M. Lo

Experimental

The Schiff base ligand was prepared by the condensation reaction of 3-hydroxy-2-naphthoyl hydrazide with 5-bromosalicylaldehyde. The title compound was prepared from the equimolar reaction of the prepared Schiff base (0.74 g, 2.0 mmol) and dicyclohexyltin oxide (0.60 g, 2.0 mmol) in toluene. The solution was left for recrystallization for a week during which yellow crystals were obtained.

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 $U(H)$ set to 1.2–1.5 times $U_{eq}(C)$. The hydroxy-H was refined with a restraint of 0.84 ± 0.01 Å. There is a high peak near the tin atom.

Figures

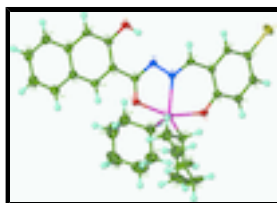


Fig. 1. The molecular structure of [*N'*-(5-bromo-2-oxidobenzylidene- κ O)-3-hydroxy-2-naphthohydrazidato- κ^2 *N',O*]dicyclohexyltin(IV) showing 50% probability displacement ellipsoids and the atom numbering. Hydrogen atoms are drawn as spheres of arbitrary radius.

[*N'*-(5-Bromo-2-oxidobenzylidene- κ O)-3-hydroxy-2-naphthohydrazidato- κ^2 *N',O*]dicyclohexyltin(IV)

Crystal data

[Sn(C₆H₁₁)₂(C₁₈H₁₁BrN₂O₃)]

$M_r = 668.18$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.2442$ (2) Å

$b = 9.9949$ (2) Å

$c = 29.6493$ (5) Å

$\beta = 94.874$ (1)°

$V = 2729.54$ (9) Å³

$Z = 4$

$F(000) = 1344$

$D_x = 1.626$ Mg m⁻³

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

Cell parameters from 9975 reflections

$\theta = 2.2$ – 30.4 °

$\mu = 2.43$ mm⁻¹

$T = 140$ K

Block, yellow

$0.33 \times 0.30 \times 0.14$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer	4787 independent reflections
Radiation source: fine-focus sealed tube graphite	4103 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.027$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.4^\circ$
$T_{\text{min}} = 0.501$, $T_{\text{max}} = 0.727$	$h = -10 \rightarrow 10$
20482 measured reflections	$k = -11 \rightarrow 11$
	$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.079$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 5.7701P]$
4787 reflections	where $P = (F_o^2 + 2F_c^2)/3$
335 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
1 restraint	$\Delta\rho_{\text{max}} = 1.60 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.49 \text{ e } \text{\AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.59441 (3)	0.67684 (3)	0.089632 (8)	0.02876 (9)
Br1	1.11466 (6)	0.10654 (5)	0.162837 (16)	0.04959 (14)
N1	0.7471 (3)	0.6588 (3)	0.14945 (9)	0.0258 (7)
N2	0.7616 (3)	0.7713 (3)	0.17740 (10)	0.0285 (7)
O1	0.6597 (3)	0.4803 (3)	0.07780 (9)	0.0414 (7)
O2	0.5924 (3)	0.8642 (3)	0.12543 (8)	0.0324 (6)

O3	0.8900 (3)	0.9235 (3)	0.23968 (9)	0.0402 (7)
H3	0.8703	0.8519	0.2256	0.060*
C1	0.8416 (4)	0.4343 (4)	0.13884 (12)	0.0268 (8)
C2	0.7606 (4)	0.4016 (4)	0.09761 (12)	0.0318 (9)
C3	0.7907 (5)	0.2795 (4)	0.07729 (14)	0.0426 (11)
H3A	0.7378	0.2555	0.0496	0.051*
C4	0.8943 (5)	0.1934 (4)	0.09617 (14)	0.0414 (10)
H4	0.9133	0.1114	0.0816	0.050*
C5	0.9709 (5)	0.2270 (4)	0.13655 (13)	0.0345 (9)
C6	0.9463 (4)	0.3444 (4)	0.15792 (12)	0.0291 (9)
H6	1.0001	0.3655	0.1858	0.035*
C7	0.8270 (4)	0.5570 (4)	0.16245 (12)	0.0267 (8)
H7	0.8819	0.5652	0.1909	0.032*
C9	0.6882 (4)	0.9979 (4)	0.18743 (11)	0.0252 (8)
C10	0.7946 (4)	1.0198 (4)	0.22456 (11)	0.0286 (8)
C11	0.8030 (4)	1.1420 (4)	0.24509 (13)	0.0343 (9)
H11	0.8773	1.1573	0.2687	0.041*
C12	0.7055 (4)	1.2460 (4)	0.23257 (12)	0.0301 (9)
C13	0.7133 (5)	1.3727 (4)	0.25347 (13)	0.0382 (10)
H13	0.7882	1.3899	0.2767	0.046*
C14	0.6160 (5)	1.4713 (4)	0.24113 (14)	0.0405 (10)
H14	0.6235	1.5561	0.2556	0.049*
C15	0.5039 (5)	1.4469 (4)	0.20675 (14)	0.0415 (10)
H15	0.4342	1.5146	0.1988	0.050*
C16	0.4952 (5)	1.3271 (4)	0.18494 (14)	0.0374 (9)
H16	0.4203	1.3128	0.1614	0.045*
C17	0.5959 (4)	1.2233 (4)	0.19668 (12)	0.0280 (8)
C18	0.5929 (4)	1.0984 (4)	0.17489 (12)	0.0283 (8)
H18	0.5216	1.0832	0.1504	0.034*
C8	0.6791 (4)	0.8710 (4)	0.16197 (11)	0.0251 (8)
C19	0.3711 (4)	0.6283 (4)	0.09615 (13)	0.0349 (9)
H19	0.3689	0.5390	0.1113	0.042*
C20	0.2916 (6)	0.6136 (7)	0.04918 (17)	0.0764 (19)
H20A	0.3390	0.5432	0.0321	0.092*
H20B	0.2973	0.6988	0.0324	0.092*
C21	0.1328 (6)	0.5768 (9)	0.0527 (2)	0.103 (3)
H21A	0.0816	0.5738	0.0220	0.124*
H21B	0.1270	0.4868	0.0663	0.124*
C22	0.0608 (6)	0.6752 (7)	0.0806 (2)	0.085 (2)
H22A	-0.0408	0.6468	0.0832	0.102*
H22B	0.0585	0.7633	0.0653	0.102*
C23	0.1366 (5)	0.6897 (6)	0.12744 (19)	0.0605 (14)
H23A	0.1297	0.6046	0.1442	0.073*
H23B	0.0881	0.7603	0.1441	0.073*
C24	0.2960 (5)	0.7263 (5)	0.12488 (17)	0.0487 (12)
H24A	0.3027	0.8172	0.1119	0.058*
H24B	0.3458	0.7274	0.1558	0.058*
C25	0.6808 (5)	0.7552 (4)	0.03016 (13)	0.0371 (10)
H25	0.7620	0.6946	0.0232	0.044*

supplementary materials

C26	0.5679 (6)	0.7490 (6)	-0.01051 (16)	0.0626 (14)
H26A	0.4844	0.8069	-0.0049	0.075*
H26B	0.5320	0.6561	-0.0146	0.075*
C27	0.6336 (8)	0.7955 (7)	-0.05379 (17)	0.084 (2)
H27A	0.7107	0.7323	-0.0611	0.101*
H27B	0.5574	0.7952	-0.0794	0.101*
C28	0.6953 (7)	0.9312 (7)	-0.0481 (2)	0.082 (2)
H28A	0.6161	0.9958	-0.0442	0.098*
H28B	0.7417	0.9564	-0.0758	0.098*
C29	0.8062 (7)	0.9396 (6)	-0.0077 (2)	0.0762 (18)
H29A	0.8397	1.0333	-0.0038	0.091*
H29B	0.8913	0.8838	-0.0133	0.091*
C30	0.7439 (6)	0.8921 (5)	0.03616 (16)	0.0553 (13)
H30A	0.8219	0.8913	0.0612	0.066*
H30B	0.6678	0.9552	0.0443	0.066*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03298 (16)	0.02502 (15)	0.02577 (14)	-0.00002 (11)	-0.01213 (10)	-0.00182 (11)
Br1	0.0606 (3)	0.0376 (3)	0.0485 (3)	0.0177 (2)	-0.0080 (2)	0.0070 (2)
N1	0.0310 (17)	0.0238 (17)	0.0212 (15)	-0.0046 (13)	-0.0053 (13)	-0.0007 (13)
N2	0.0329 (18)	0.0245 (17)	0.0263 (16)	-0.0037 (14)	-0.0078 (14)	-0.0043 (13)
O1	0.0531 (19)	0.0277 (15)	0.0383 (15)	0.0068 (13)	-0.0254 (14)	-0.0072 (12)
O2	0.0363 (16)	0.0266 (14)	0.0315 (14)	0.0019 (11)	-0.0141 (12)	-0.0044 (11)
O3	0.0490 (18)	0.0305 (16)	0.0369 (16)	0.0056 (13)	-0.0208 (13)	-0.0051 (12)
C1	0.031 (2)	0.024 (2)	0.0247 (18)	-0.0032 (16)	-0.0020 (16)	0.0026 (15)
C2	0.039 (2)	0.027 (2)	0.027 (2)	-0.0021 (17)	-0.0060 (17)	0.0013 (16)
C3	0.062 (3)	0.029 (2)	0.033 (2)	0.002 (2)	-0.018 (2)	-0.0063 (18)
C4	0.061 (3)	0.024 (2)	0.037 (2)	0.006 (2)	-0.007 (2)	-0.0030 (18)
C5	0.045 (2)	0.026 (2)	0.031 (2)	0.0057 (18)	-0.0014 (18)	0.0083 (17)
C6	0.036 (2)	0.023 (2)	0.0270 (19)	-0.0029 (16)	-0.0042 (16)	0.0045 (15)
C7	0.027 (2)	0.029 (2)	0.0230 (18)	-0.0057 (16)	-0.0052 (15)	0.0025 (15)
C9	0.026 (2)	0.029 (2)	0.0208 (17)	-0.0051 (16)	0.0018 (14)	0.0009 (15)
C10	0.033 (2)	0.031 (2)	0.0209 (18)	0.0002 (17)	-0.0036 (15)	-0.0003 (16)
C11	0.037 (2)	0.037 (2)	0.028 (2)	-0.0048 (18)	-0.0068 (17)	-0.0050 (17)
C12	0.036 (2)	0.030 (2)	0.0255 (19)	-0.0042 (17)	0.0067 (16)	-0.0026 (16)
C13	0.050 (3)	0.036 (2)	0.027 (2)	-0.005 (2)	0.0008 (19)	-0.0052 (18)
C14	0.058 (3)	0.031 (2)	0.035 (2)	0.001 (2)	0.014 (2)	-0.0080 (18)
C15	0.047 (3)	0.037 (2)	0.041 (2)	0.010 (2)	0.009 (2)	-0.002 (2)
C16	0.036 (2)	0.036 (2)	0.039 (2)	0.0025 (19)	0.0006 (18)	0.0014 (19)
C17	0.030 (2)	0.029 (2)	0.0263 (19)	-0.0028 (16)	0.0071 (16)	0.0012 (16)
C18	0.027 (2)	0.032 (2)	0.0254 (19)	-0.0038 (16)	-0.0007 (15)	-0.0006 (16)
C8	0.0224 (19)	0.032 (2)	0.0208 (18)	-0.0048 (16)	-0.0011 (15)	0.0014 (15)
C19	0.034 (2)	0.033 (2)	0.036 (2)	-0.0056 (18)	-0.0085 (18)	0.0028 (18)
C20	0.048 (3)	0.138 (6)	0.041 (3)	-0.035 (3)	-0.008 (2)	-0.012 (3)
C21	0.054 (4)	0.203 (9)	0.050 (3)	-0.063 (5)	-0.011 (3)	-0.016 (4)
C22	0.032 (3)	0.128 (6)	0.092 (5)	-0.011 (3)	-0.012 (3)	0.070 (4)

C23	0.044 (3)	0.056 (3)	0.082 (4)	-0.002 (2)	0.004 (3)	0.006 (3)
C24	0.041 (3)	0.041 (3)	0.064 (3)	-0.007 (2)	0.005 (2)	-0.002 (2)
C25	0.043 (3)	0.039 (2)	0.028 (2)	0.005 (2)	-0.0009 (18)	0.0019 (18)
C26	0.072 (4)	0.072 (4)	0.042 (3)	-0.009 (3)	-0.010 (3)	0.004 (3)
C27	0.100 (5)	0.117 (6)	0.033 (3)	-0.009 (4)	-0.002 (3)	0.006 (3)
C28	0.083 (4)	0.095 (5)	0.069 (4)	0.006 (4)	0.010 (3)	0.042 (4)
C29	0.095 (5)	0.061 (4)	0.076 (4)	-0.017 (3)	0.026 (4)	0.003 (3)
C30	0.066 (3)	0.050 (3)	0.050 (3)	-0.010 (3)	0.002 (2)	-0.003 (2)

Geometric parameters (Å, °)

Sn1—O1	2.094 (3)	C16—C17	1.418 (6)
Sn1—C25	2.145 (4)	C16—H16	0.9500
Sn1—C19	2.145 (4)	C17—C18	1.405 (5)
Sn1—O2	2.153 (3)	C18—H18	0.9500
Sn1—N1	2.178 (3)	C19—C24	1.506 (6)
Br1—C5	1.910 (4)	C19—C20	1.525 (6)
N1—C7	1.296 (5)	C19—H19	1.0000
N1—N2	1.397 (4)	C20—C21	1.525 (7)
N2—C8	1.313 (5)	C20—H20A	0.9900
O1—C2	1.319 (5)	C20—H20B	0.9900
O2—C8	1.294 (4)	C21—C22	1.480 (10)
O3—C10	1.356 (4)	C21—H21A	0.9900
O3—H3	0.8400	C21—H21B	0.9900
C1—C6	1.404 (5)	C22—C23	1.507 (8)
C1—C2	1.416 (5)	C22—H22A	0.9900
C1—C7	1.425 (5)	C22—H22B	0.9900
C2—C3	1.399 (6)	C23—C24	1.527 (6)
C3—C4	1.371 (6)	C23—H23A	0.9900
C3—H3A	0.9500	C23—H23B	0.9900
C4—C5	1.380 (6)	C24—H24A	0.9900
C4—H4	0.9500	C24—H24B	0.9900
C5—C6	1.362 (5)	C25—C30	1.492 (6)
C6—H6	0.9500	C25—C26	1.527 (6)
C7—H7	0.9500	C25—H25	1.0000
C9—C18	1.367 (5)	C26—C27	1.537 (7)
C9—C10	1.429 (5)	C26—H26A	0.9900
C9—C8	1.475 (5)	C26—H26B	0.9900
C10—C11	1.364 (5)	C27—C28	1.476 (9)
C11—C12	1.404 (6)	C27—H27A	0.9900
C11—H11	0.9500	C27—H27B	0.9900
C12—C13	1.409 (6)	C28—C29	1.513 (8)
C12—C17	1.424 (5)	C28—H28A	0.9900
C13—C14	1.363 (6)	C28—H28B	0.9900
C13—H13	0.9500	C29—C30	1.540 (7)
C14—C15	1.411 (6)	C29—H29A	0.9900
C14—H14	0.9500	C29—H29B	0.9900
C15—C16	1.360 (6)	C30—H30A	0.9900
C15—H15	0.9500	C30—H30B	0.9900

supplementary materials

O1—Sn1—C25	94.14 (15)	C24—C19—Sn1	113.4 (3)
O1—Sn1—C19	95.51 (14)	C20—C19—Sn1	109.4 (3)
C25—Sn1—C19	125.81 (15)	C24—C19—H19	107.4
O1—Sn1—O2	155.97 (9)	C20—C19—H19	107.4
C25—Sn1—O2	96.14 (14)	Sn1—C19—H19	107.4
C19—Sn1—O2	95.96 (13)	C19—C20—C21	110.7 (4)
O1—Sn1—N1	83.25 (10)	C19—C20—H20A	109.5
C25—Sn1—N1	116.02 (14)	C21—C20—H20A	109.5
C19—Sn1—N1	118.03 (13)	C19—C20—H20B	109.5
O2—Sn1—N1	72.71 (10)	C21—C20—H20B	109.5
C7—N1—N2	115.6 (3)	H20A—C20—H20B	108.1
C7—N1—Sn1	128.4 (2)	C22—C21—C20	111.0 (6)
N2—N1—Sn1	116.1 (2)	C22—C21—H21A	109.4
C8—N2—N1	112.4 (3)	C20—C21—H21A	109.4
C2—O1—Sn1	133.4 (2)	C22—C21—H21B	109.4
C8—O2—Sn1	115.3 (2)	C20—C21—H21B	109.4
C10—O3—H3	109.5	H21A—C21—H21B	108.0
C6—C1—C2	119.7 (3)	C21—C22—C23	112.6 (5)
C6—C1—C7	116.4 (3)	C21—C22—H22A	109.1
C2—C1—C7	123.9 (3)	C23—C22—H22A	109.1
O1—C2—C3	119.1 (3)	C21—C22—H22B	109.1
O1—C2—C1	123.3 (3)	C23—C22—H22B	109.1
C3—C2—C1	117.6 (3)	H22A—C22—H22B	107.8
C4—C3—C2	121.9 (4)	C22—C23—C24	110.6 (4)
C4—C3—H3A	119.0	C22—C23—H23A	109.5
C2—C3—H3A	119.0	C24—C23—H23A	109.5
C3—C4—C5	119.4 (4)	C22—C23—H23B	109.5
C3—C4—H4	120.3	C24—C23—H23B	109.5
C5—C4—H4	120.3	H23A—C23—H23B	108.1
C6—C5—C4	121.3 (4)	C19—C24—C23	111.5 (4)
C6—C5—Br1	119.4 (3)	C19—C24—H24A	109.3
C4—C5—Br1	119.3 (3)	C23—C24—H24A	109.3
C5—C6—C1	120.0 (3)	C19—C24—H24B	109.3
C5—C6—H6	120.0	C23—C24—H24B	109.3
C1—C6—H6	120.0	H24A—C24—H24B	108.0
N1—C7—C1	127.2 (3)	C30—C25—C26	111.4 (4)
N1—C7—H7	116.4	C30—C25—Sn1	114.0 (3)
C1—C7—H7	116.4	C26—C25—Sn1	110.9 (3)
C18—C9—C10	118.8 (3)	C30—C25—H25	106.7
C18—C9—C8	119.1 (3)	C26—C25—H25	106.7
C10—C9—C8	122.1 (3)	Sn1—C25—H25	106.7
O3—C10—C11	118.5 (3)	C25—C26—C27	110.8 (4)
O3—C10—C9	122.1 (3)	C25—C26—H26A	109.5
C11—C10—C9	119.3 (3)	C27—C26—H26A	109.5
C10—C11—C12	122.3 (3)	C25—C26—H26B	109.5
C10—C11—H11	118.9	C27—C26—H26B	109.5
C12—C11—H11	118.9	H26A—C26—H26B	108.1
C11—C12—C13	122.8 (4)	C28—C27—C26	111.0 (5)
C11—C12—C17	118.6 (3)	C28—C27—H27A	109.4

C13—C12—C17	118.6 (4)	C26—C27—H27A	109.4
C14—C13—C12	121.6 (4)	C28—C27—H27B	109.4
C14—C13—H13	119.2	C26—C27—H27B	109.4
C12—C13—H13	119.2	H27A—C27—H27B	108.0
C13—C14—C15	119.8 (4)	C27—C28—C29	111.8 (5)
C13—C14—H14	120.1	C27—C28—H28A	109.3
C15—C14—H14	120.1	C29—C28—H28A	109.3
C16—C15—C14	120.4 (4)	C27—C28—H28B	109.3
C16—C15—H15	119.8	C29—C28—H28B	109.3
C14—C15—H15	119.8	H28A—C28—H28B	107.9
C15—C16—C17	121.1 (4)	C28—C29—C30	112.0 (5)
C15—C16—H16	119.5	C28—C29—H29A	109.2
C17—C16—H16	119.5	C30—C29—H29A	109.2
C18—C17—C16	123.4 (4)	C28—C29—H29B	109.2
C18—C17—C12	118.1 (3)	C30—C29—H29B	109.2
C16—C17—C12	118.5 (4)	H29A—C29—H29B	107.9
C9—C18—C17	122.8 (3)	C25—C30—C29	110.6 (4)
C9—C18—H18	118.6	C25—C30—H30A	109.5
C17—C18—H18	118.6	C29—C30—H30A	109.5
O2—C8—N2	123.5 (3)	C25—C30—H30B	109.5
O2—C8—C9	118.6 (3)	C29—C30—H30B	109.5
N2—C8—C9	117.9 (3)	H30A—C30—H30B	108.1
C24—C19—C20	111.7 (4)		
O1—Sn1—N1—C7	0.0 (3)	C15—C16—C17—C18	-179.2 (4)
C25—Sn1—N1—C7	-91.3 (3)	C15—C16—C17—C12	1.2 (6)
C19—Sn1—N1—C7	92.7 (3)	C11—C12—C17—C18	-1.4 (5)
O2—Sn1—N1—C7	-179.8 (3)	C13—C12—C17—C18	177.5 (4)
O1—Sn1—N1—N2	179.7 (3)	C11—C12—C17—C16	178.3 (4)
C25—Sn1—N1—N2	88.4 (3)	C13—C12—C17—C16	-2.9 (5)
C19—Sn1—N1—N2	-87.6 (3)	C10—C9—C18—C17	0.7 (6)
O2—Sn1—N1—N2	0.0 (2)	C8—C9—C18—C17	-178.6 (3)
C7—N1—N2—C8	179.2 (3)	C16—C17—C18—C9	-178.1 (4)
Sn1—N1—N2—C8	-0.6 (4)	C12—C17—C18—C9	1.5 (6)
C25—Sn1—O1—C2	109.0 (4)	Sn1—O2—C8—N2	-1.3 (5)
C19—Sn1—O1—C2	-124.4 (4)	Sn1—O2—C8—C9	177.7 (2)
O2—Sn1—O1—C2	-6.2 (6)	N1—N2—C8—O2	1.3 (5)
N1—Sn1—O1—C2	-6.8 (4)	N1—N2—C8—C9	-177.7 (3)
O1—Sn1—O2—C8	0.1 (4)	C18—C9—C8—O2	7.8 (5)
C25—Sn1—O2—C8	-114.7 (3)	C10—C9—C8—O2	-171.5 (3)
C19—Sn1—O2—C8	118.2 (3)	C18—C9—C8—N2	-173.2 (3)
N1—Sn1—O2—C8	0.7 (2)	C10—C9—C8—N2	7.5 (5)
Sn1—O1—C2—C3	-171.0 (3)	O1—Sn1—C19—C24	153.9 (3)
Sn1—O1—C2—C1	8.8 (6)	C25—Sn1—C19—C24	-106.9 (3)
C6—C1—C2—O1	179.4 (4)	O2—Sn1—C19—C24	-4.9 (3)
C7—C1—C2—O1	-2.4 (6)	N1—Sn1—C19—C24	68.6 (3)
C6—C1—C2—C3	-0.7 (6)	O1—Sn1—C19—C20	-80.7 (4)
C7—C1—C2—C3	177.5 (4)	C25—Sn1—C19—C20	18.4 (4)
O1—C2—C3—C4	179.9 (4)	O2—Sn1—C19—C20	120.4 (4)
C1—C2—C3—C4	0.1 (7)	N1—Sn1—C19—C20	-166.0 (4)

supplementary materials

C2—C3—C4—C5	0.5 (7)	C24—C19—C20—C21	-54.5 (7)
C3—C4—C5—C6	-0.4 (7)	Sn1—C19—C20—C21	179.1 (5)
C3—C4—C5—Br1	179.8 (4)	C19—C20—C21—C22	55.3 (8)
C4—C5—C6—C1	-0.2 (6)	C20—C21—C22—C23	-56.7 (7)
Br1—C5—C6—C1	179.6 (3)	C21—C22—C23—C24	55.8 (7)
C2—C1—C6—C5	0.8 (6)	C20—C19—C24—C23	54.3 (5)
C7—C1—C6—C5	-177.5 (4)	Sn1—C19—C24—C23	178.4 (3)
N2—N1—C7—C1	-175.0 (3)	C22—C23—C24—C19	-54.0 (6)
Sn1—N1—C7—C1	4.7 (6)	O1—Sn1—C25—C30	-143.8 (3)
C6—C1—C7—N1	173.8 (4)	C19—Sn1—C25—C30	116.3 (3)
C2—C1—C7—N1	-4.4 (6)	O2—Sn1—C25—C30	14.4 (3)
C18—C9—C10—O3	178.2 (4)	N1—Sn1—C25—C30	-59.3 (4)
C8—C9—C10—O3	-2.5 (6)	O1—Sn1—C25—C26	89.5 (3)
C18—C9—C10—C11	-3.1 (6)	C19—Sn1—C25—C26	-10.4 (4)
C8—C9—C10—C11	176.2 (4)	O2—Sn1—C25—C26	-112.3 (3)
O3—C10—C11—C12	-177.9 (4)	N1—Sn1—C25—C26	174.0 (3)
C9—C10—C11—C12	3.4 (6)	C30—C25—C26—C27	56.1 (6)
C10—C11—C12—C13	-179.9 (4)	Sn1—C25—C26—C27	-175.8 (4)
C10—C11—C12—C17	-1.1 (6)	C25—C26—C27—C28	-56.2 (7)
C11—C12—C13—C14	-179.0 (4)	C26—C27—C28—C29	55.7 (8)
C17—C12—C13—C14	2.2 (6)	C27—C28—C29—C30	-54.9 (8)
C12—C13—C14—C15	0.2 (6)	C26—C25—C30—C29	-54.8 (6)
C13—C14—C15—C16	-2.0 (6)	Sn1—C25—C30—C29	178.8 (4)
C14—C15—C16—C17	1.3 (6)	C28—C29—C30—C25	54.1 (7)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots N2	0.84	1.86	2.600 (4)	146

Fig. 1

