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

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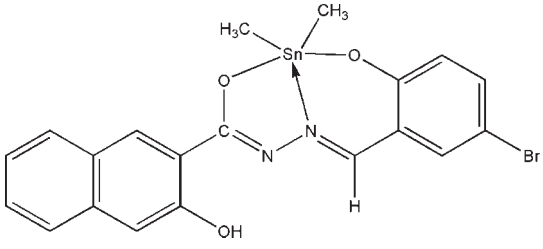
Key indicators: single-crystal X-ray study; T = 145 K; mean σ(C–C) = 0.005 Å; R factor = 0.024; wR factor = 0.079; data-to-parameter ratio = 16.4.

The Sn^{IV} atom in the title compound, [Sn(CH$_3$)$_2$-(C$_{18}$H$_{11}$BrN$_2$O$_3$)], shows a distorted *cis*-C$_2$NO$_2$Sn trigonal-bipyramidal coordination geometry, with an axial O—Sn—O angle of 155.27 (9)°. The presence of an intramolecular O—H···N hydrogen bond between the amido N atom and hydroxy H atom in the Schiff base ligand helps to stabilize the overall molecular structure.

Related literature

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



Experimental

Crystal data

[Sn(CH$_3$)$_2$(C$_{18}$H$_{11}$BrN$_2$O$_3$)] M_r = 531.96
Triclinic, $P\overline{1}$
a = 6.8662 (5) Å
b = 11.7998 (9) Å
c = 11.9365 (9) Å
α = 87.464 (1)°
β = 76.128 (1)°
γ = 81.213 (1)°
V = 927.84 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.55 mm^{-1}
T = 145 K
0.39 × 0.37 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.338, T_{max} = 0.740
5350 measured reflections
4028 independent reflections
3703 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.079
S = 1.14
4028 reflections
245 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···N2	0.84	1.88	2.611 (4)	144

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 20080); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2691).

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supporting information

Acta Cryst. (2010). E**66**, m161 [https://doi.org/10.1107/S1600536810001133]

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

See Mun Lee, Hapipah Mohd Ali and Kong Mun Lo

S1. Experimental

The Schiff base ligand was prepared by the condensation reaction of 3-hydroxy-2-naphthoyl hydrazide with 5-bromo-salicylaldehyde. The title compound was prepared by refluxing the Schiff base (0.74 g, 2.0 mmol) with dimethyltin oxide (0.32 g, 2.0 mmol) in toluene for 6 h. The solution was filtered and left for recrystallization for a week during which yellow crystals were obtained.

S2. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C-H) = 0.95Å, U_{iso}=1.2U_{eq} (C) for aromatic 0.98Å, U_{iso} = 1.5U_{eq} (C) for CH_3 atoms and 0.84Å, U_{iso} = 1.5U_{eq} (O) for the OH group.

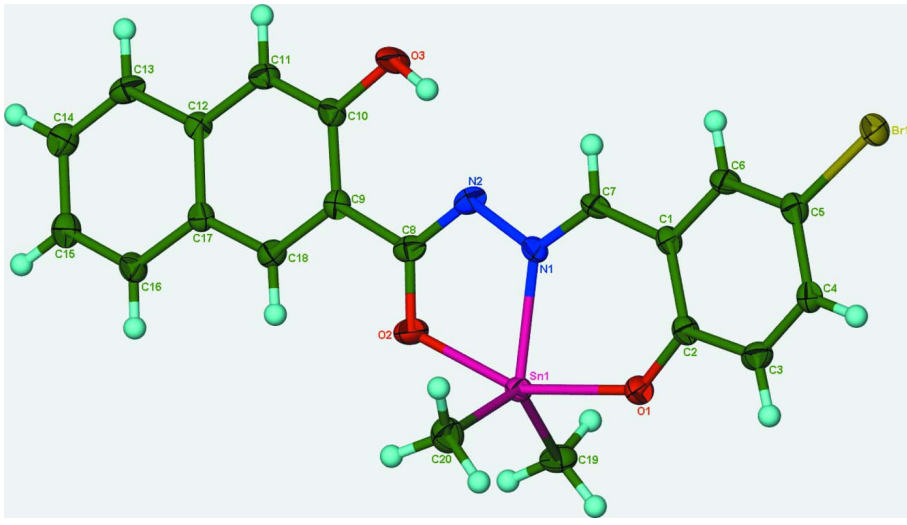

Figure 1

The molecular structure of [*N*′-(5-bromo-2-oxidobenzylidene-κ*O*)-3-hydroxy-2- naphthohydrazidato-κ^2*N*′,*O*]dimethyltin(IV) showing 70% 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*]dimethyltin(IV)

Crystal data

$[Sn(CH_3)_2(C_{18}H_{11}BrN_2O_3)]$
M_r = 531.96
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.8662 (5) Å
b = 11.7998 (9) Å

c = 11.9365 (9) Å
α = 87.464 (1)°
β = 76.128 (1)°
γ = 81.213 (1)°
V = 927.84 (12) Å^3
Z = 2
F(000) = 520
D_x = 1.904 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3900 reflections
θ = 2.5–30.6°
μ = 3.55 mm^{-1}
T = 145 K
Plate, yellow
0.39 × 0.37 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.338, T_{max} = 0.740

5350 measured reflections
4028 independent reflections
3703 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −8→8
k = −10→15
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.079
S = 1.14
4028 reflections
245 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 1.8608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.75049 (3)	0.561594 (19)	0.670242 (18)	0.01412 (8)
Br1	0.57215 (5)	−0.06224 (3)	0.64595 (3)	0.02011 (9)
N1	0.5307 (4)	0.4692 (2)	0.7889 (2)	0.0141 (5)
N2	0.3995 (4)	0.5332 (3)	0.8788 (2)	0.0172 (6)
O1	0.8546 (4)	0.4001 (2)	0.5966 (2)	0.0202 (5)
O2	0.5723 (4)	0.6809 (2)	0.7987 (2)	0.0228 (5)
O3	0.1095 (4)	0.5698 (2)	1.0656 (2)	0.0219 (5)
H3	0.1750	0.5344	1.0054	0.033*
C1	0.6138 (5)	0.2791 (3)	0.6996 (3)	0.0141 (6)

C2	0.7792 (5)	0.3027 (3)	0.6092 (3)	0.0152 (6)
C3	0.8681 (5)	0.2152 (3)	0.5277 (3)	0.0188 (7)
H3A	0.9776	0.2288	0.4655	0.023*
C4	0.7999 (5)	0.1105 (3)	0.5364 (3)	0.0158 (6)
H4	0.8593	0.0541	0.4790	0.019*
C5	0.6435 (5)	0.0871 (3)	0.6295 (3)	0.0164 (6)
C6	0.5524 (5)	0.1702 (3)	0.7093 (3)	0.0154 (6)
H6	0.4459	0.1540	0.7723	0.019*
C7	0.5032 (5)	0.3630 (3)	0.7853 (3)	0.0150 (6)
H7	0.3999	0.3379	0.8450	0.018*
C8	0.4332 (5)	0.6410 (3)	0.8761 (3)	0.0164 (6)
C9	0.3027 (5)	0.7184 (3)	0.9668 (3)	0.0151 (6)
C10	0.1483 (5)	0.6797 (3)	1.0581 (3)	0.0147 (6)
C11	0.0383 (5)	0.7555 (3)	1.1419 (3)	0.0154 (6)
H11	−0.0602	0.7291	1.2037	0.018*
C12	0.0673 (5)	0.8711 (3)	1.1392 (3)	0.0139 (6)
C13	−0.0460 (5)	0.9515 (3)	1.2244 (3)	0.0189 (7)
H13	−0.1429	0.9267	1.2880	0.023*
C14	−0.0175 (5)	1.0647 (3)	1.2160 (3)	0.0190 (7)
H14	−0.0962	1.1174	1.2732	0.023*
C15	0.1279 (5)	1.1033 (3)	1.1232 (3)	0.0192 (7)
H15	0.1469	1.1816	1.1186	0.023*
C16	0.2407 (5)	1.0289 (3)	1.0405 (3)	0.0164 (6)
H16	0.3376	1.0558	0.9782	0.020*
C17	0.2153 (5)	0.9112 (3)	1.0461 (3)	0.0138 (6)
C18	0.3312 (5)	0.8320 (3)	0.9627 (3)	0.0152 (6)
H18	0.4322	0.8573	0.9017	0.018*
C19	1.0295 (5)	0.5826 (3)	0.7067 (3)	0.0201 (7)
H19A	1.0478	0.5367	0.7748	0.030*
H19B	1.0291	0.6637	0.7216	0.030*
H19C	1.1409	0.5572	0.6405	0.030*
C20	0.6241 (5)	0.6376 (3)	0.5344 (3)	0.0227 (7)
H20A	0.4933	0.6117	0.5391	0.034*
H20B	0.7165	0.6150	0.4601	0.034*
H20C	0.6040	0.7213	0.5412	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01425 (12)	0.01281 (13)	0.01497 (12)	−0.00358 (8)	−0.00180 (8)	−0.00023 (8)
Br1	0.02169 (17)	0.01283 (18)	0.02579 (18)	−0.00506 (13)	−0.00342 (14)	−0.00316 (13)
N1	0.0149 (12)	0.0107 (13)	0.0174 (13)	−0.0042 (10)	−0.0034 (10)	0.0001 (10)
N2	0.0154 (13)	0.0220 (15)	0.0131 (12)	−0.0028 (11)	−0.0010 (10)	−0.0018 (11)
O1	0.0197 (12)	0.0140 (12)	0.0244 (12)	−0.0038 (9)	0.0011 (10)	−0.0017 (10)
O2	0.0216 (12)	0.0197 (13)	0.0232 (12)	−0.0073 (10)	0.0054 (10)	−0.0029 (10)
O3	0.0292 (13)	0.0127 (12)	0.0214 (12)	−0.0114 (10)	0.0050 (10)	−0.0056 (9)
C1	0.0160 (14)	0.0122 (15)	0.0151 (14)	−0.0024 (12)	−0.0058 (12)	−0.0001 (12)
C2	0.0162 (15)	0.0134 (16)	0.0172 (15)	−0.0026 (12)	−0.0061 (12)	0.0000 (12)

C3	0.0164 (15)	0.0223 (18)	0.0160 (15)	−0.0008 (13)	−0.0022 (12)	0.0031 (13)
C4	0.0175 (15)	0.0133 (16)	0.0168 (15)	−0.0006 (12)	−0.0051 (12)	−0.0014 (12)
C5	0.0173 (15)	0.0141 (16)	0.0194 (16)	−0.0024 (12)	−0.0075 (12)	−0.0002 (13)
C6	0.0146 (14)	0.0159 (16)	0.0171 (15)	−0.0062 (12)	−0.0042 (12)	0.0015 (12)
C7	0.0157 (14)	0.0140 (16)	0.0168 (15)	−0.0063 (12)	−0.0049 (12)	0.0033 (12)
C8	0.0131 (14)	0.0223 (18)	0.0143 (15)	−0.0037 (12)	−0.0040 (12)	0.0021 (13)
C9	0.0151 (14)	0.0150 (16)	0.0157 (15)	−0.0012 (12)	−0.0051 (12)	−0.0013 (12)
C10	0.0181 (15)	0.0119 (15)	0.0155 (15)	−0.0045 (12)	−0.0047 (12)	−0.0025 (12)
C11	0.0154 (14)	0.0174 (17)	0.0139 (14)	−0.0057 (12)	−0.0024 (12)	−0.0015 (12)
C12	0.0139 (14)	0.0144 (16)	0.0149 (14)	−0.0036 (12)	−0.0050 (11)	−0.0022 (12)
C13	0.0145 (15)	0.0284 (19)	0.0137 (15)	−0.0037 (13)	−0.0029 (12)	0.0001 (13)
C14	0.0202 (16)	0.0201 (18)	0.0178 (16)	−0.0024 (13)	−0.0059 (13)	−0.0044 (13)
C15	0.0207 (16)	0.0173 (17)	0.0206 (16)	−0.0011 (13)	−0.0073 (13)	−0.0035 (13)
C16	0.0182 (15)	0.0120 (16)	0.0202 (16)	−0.0047 (12)	−0.0051 (12)	−0.0025 (12)
C17	0.0162 (14)	0.0134 (15)	0.0125 (14)	−0.0016 (12)	−0.0049 (11)	−0.0024 (12)
C18	0.0147 (14)	0.0176 (17)	0.0132 (14)	−0.0020 (12)	−0.0035 (11)	−0.0007 (12)
C19	0.0173 (15)	0.0249 (19)	0.0193 (16)	−0.0090 (14)	−0.0031 (13)	−0.0007 (14)
C20	0.0225 (17)	0.0223 (19)	0.0238 (17)	−0.0015 (14)	−0.0079 (14)	0.0017 (14)

Geometric parameters (Å, º)

Sn1—O1	2.084 (2)	C8—C9	1.477 (5)
Sn1—C19	2.116 (3)	C9—C18	1.381 (5)
Sn1—C20	2.120 (3)	C9—C10	1.438 (4)
Sn1—O2	2.143 (2)	C10—C11	1.372 (5)
Sn1—N1	2.194 (3)	C11—C12	1.406 (5)
Br1—C5	1.890 (3)	C11—H11	0.9500
N1—C7	1.300 (4)	C12—C13	1.421 (5)
N1—N2	1.390 (4)	C12—C17	1.432 (4)
N2—C8	1.324 (5)	C13—C14	1.375 (5)
O1—C2	1.320 (4)	C13—H13	0.9500
O2—C8	1.290 (4)	C14—C15	1.412 (5)
O3—C10	1.358 (4)	C14—H14	0.9500
O3—H3	0.8400	C15—C16	1.360 (5)
C1—C6	1.404 (4)	C15—H15	0.9500
C1—C2	1.419 (4)	C16—C17	1.422 (5)
C1—C7	1.446 (5)	C16—H16	0.9500
C2—C3	1.413 (5)	C17—C18	1.405 (4)
C3—C4	1.377 (5)	C18—H18	0.9500
C3—H3A	0.9500	C19—H19A	0.9800
C4—C5	1.399 (5)	C19—H19B	0.9800
C4—H4	0.9500	C19—H19C	0.9800
C5—C6	1.367 (5)	C20—H20A	0.9800
C6—H6	0.9500	C20—H20B	0.9800
C7—H7	0.9500	C20—H20C	0.9800
O1—Sn1—C19	95.10 (12)	C18—C9—C8	118.2 (3)
O1—Sn1—C20	97.09 (13)	C10—C9—C8	122.5 (3)

C19—Sn1—C20	127.84 (14)	O3—C10—C11	118.6 (3)
O1—Sn1—O2	155.27 (9)	O3—C10—C9	122.3 (3)
C19—Sn1—O2	94.33 (12)	C11—C10—C9	119.2 (3)
C20—Sn1—O2	95.04 (13)	C10—C11—C12	121.9 (3)
O1—Sn1—N1	83.01 (10)	C10—C11—H11	119.0
C19—Sn1—N1	121.63 (12)	C12—C11—H11	119.0
C20—Sn1—N1	110.12 (12)	C11—C12—C13	123.0 (3)
O2—Sn1—N1	72.59 (10)	C11—C12—C17	119.2 (3)
C7—N1—N2	115.3 (3)	C13—C12—C17	117.8 (3)
C7—N1—Sn1	128.8 (2)	C14—C13—C12	121.0 (3)
N2—N1—Sn1	115.9 (2)	C14—C13—H13	119.5
C8—N2—N1	112.2 (3)	C12—C13—H13	119.5
C2—O1—Sn1	133.1 (2)	C13—C14—C15	120.6 (3)
C8—O2—Sn1	115.9 (2)	C13—C14—H14	119.7
C10—O3—H3	109.5	C15—C14—H14	119.7
C6—C1—C2	120.1 (3)	C16—C15—C14	120.3 (3)
C6—C1—C7	117.1 (3)	C16—C15—H15	119.9
C2—C1—C7	122.8 (3)	C14—C15—H15	119.9
O1—C2—C3	118.3 (3)	C15—C16—C17	120.7 (3)
O1—C2—C1	124.5 (3)	C15—C16—H16	119.6
C3—C2—C1	117.2 (3)	C17—C16—H16	119.6
C4—C3—C2	121.6 (3)	C18—C17—C16	122.1 (3)
C4—C3—H3A	119.2	C18—C17—C12	118.3 (3)
C2—C3—H3A	119.2	C16—C17—C12	119.6 (3)
C3—C4—C5	120.2 (3)	C9—C18—C17	121.9 (3)
C3—C4—H4	119.9	C9—C18—H18	119.0
C5—C4—H4	119.9	C17—C18—H18	119.0
C6—C5—C4	119.8 (3)	Sn1—C19—H19A	109.5
C6—C5—Br1	121.4 (2)	Sn1—C19—H19B	109.5
C4—C5—Br1	118.7 (3)	H19A—C19—H19B	109.5
C5—C6—C1	120.9 (3)	Sn1—C19—H19C	109.5
C5—C6—H6	119.5	H19A—C19—H19C	109.5
C1—C6—H6	119.5	H19B—C19—H19C	109.5
N1—C7—C1	126.6 (3)	Sn1—C20—H20A	109.5
N1—C7—H7	116.7	Sn1—C20—H20B	109.5
C1—C7—H7	116.7	H20A—C20—H20B	109.5
O2—C8—N2	123.4 (3)	Sn1—C20—H20C	109.5
O2—C8—C9	119.1 (3)	H20A—C20—H20C	109.5
N2—C8—C9	117.5 (3)	H20B—C20—H20C	109.5
C18—C9—C10	119.4 (3)		

O1—Sn1—N1—C7	−5.4 (3)	Sn1—N1—C7—C1	−0.2 (5)
C19—Sn1—N1—C7	−97.1 (3)	C6—C1—C7—N1	−177.1 (3)
C20—Sn1—N1—C7	89.6 (3)	C2—C1—C7—N1	3.5 (5)
O2—Sn1—N1—C7	178.6 (3)	Sn1—O2—C8—N2	0.3 (4)
O1—Sn1—N1—N2	176.3 (2)	Sn1—O2—C8—C9	−179.4 (2)
C19—Sn1—N1—N2	84.6 (2)	N1—N2—C8—O2	0.0 (4)
C20—Sn1—N1—N2	−88.7 (2)	N1—N2—C8—C9	179.6 (3)

O2—Sn1—N1—N2	0.3 (2)	O2—C8—C9—C18	2.0 (4)
C7—N1—N2—C8	−178.8 (3)	N2—C8—C9—C18	−177.7 (3)
Sn1—N1—N2—C8	−0.3 (3)	O2—C8—C9—C10	−178.2 (3)
C19—Sn1—O1—C2	133.7 (3)	N2—C8—C9—C10	2.2 (5)
C20—Sn1—O1—C2	−97.1 (3)	C18—C9—C10—O3	178.5 (3)
O2—Sn1—O1—C2	21.7 (4)	C8—C9—C10—O3	−1.4 (5)
N1—Sn1—O1—C2	12.4 (3)	C18—C9—C10—C11	−2.7 (5)
O1—Sn1—O2—C8	−10.0 (4)	C8—C9—C10—C11	177.4 (3)
C19—Sn1—O2—C8	−122.1 (2)	O3—C10—C11—C12	−178.9 (3)
C20—Sn1—O2—C8	109.2 (2)	C9—C10—C11—C12	2.2 (5)
N1—Sn1—O2—C8	−0.3 (2)	C10—C11—C12—C13	179.4 (3)
Sn1—O1—C2—C3	166.5 (2)	C10—C11—C12—C17	0.2 (5)
Sn1—O1—C2—C1	−13.5 (5)	C11—C12—C13—C14	−177.7 (3)
C6—C1—C2—O1	−176.3 (3)	C17—C12—C13—C14	1.5 (5)
C7—C1—C2—O1	3.1 (5)	C12—C13—C14—C15	−1.0 (5)
C6—C1—C2—C3	3.7 (4)	C13—C14—C15—C16	0.4 (5)
C7—C1—C2—C3	−177.0 (3)	C14—C15—C16—C17	−0.3 (5)
O1—C2—C3—C4	178.9 (3)	C15—C16—C17—C18	−179.2 (3)
C1—C2—C3—C4	−1.1 (5)	C15—C16—C17—C12	0.9 (5)
C2—C3—C4—C5	−2.2 (5)	C11—C12—C17—C18	−2.1 (4)
C3—C4—C5—C6	2.8 (5)	C13—C12—C17—C18	178.7 (3)
C3—C4—C5—Br1	−174.0 (2)	C11—C12—C17—C16	177.8 (3)
C4—C5—C6—C1	−0.2 (5)	C13—C12—C17—C16	−1.4 (4)
Br1—C5—C6—C1	176.6 (2)	C10—C9—C18—C17	0.8 (5)
C2—C1—C6—C5	−3.1 (5)	C8—C9—C18—C17	−179.3 (3)
C7—C1—C6—C5	177.5 (3)	C16—C17—C18—C9	−178.3 (3)
N2—N1—C7—C1	178.1 (3)	C12—C17—C18—C9	1.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N2	0.84	1.88	2.611 (4)	144