Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[*N*-(5-Chloro-2-oxidobenzylidene)-valinato-κ^3O,N,O']dicyclohexyltin(IV)

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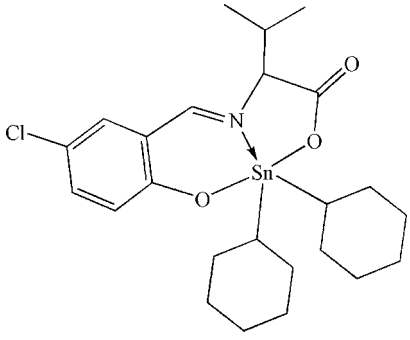
Received 23 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.047; wR factor = 0.104; data-to-parameter ratio = 16.6.

The tin atom of the title compound, $[Sn(C_6H_{11})_2(C_{12}H_{12}ClNO_3)]$, adopts a distorted $SnNC_2O_2$ trigonal–bipyramidal geometry, and forms five- and six-membered chelate rings with the tridentate ligand.

Related literature

For related literature, see: Beltran *et al.* (2003); Dakternieks *et al.* (1998); Tian *et al.* (2004, 2005, 2006, 2007).



Experimental

Crystal data

$[Sn(C_6H_{11})_2(C_{12}H_{12}ClNO_3)]$
M_r = 538.66
Monoclinic, $P2_1/n$
a = 9.9830 (18) Å
b = 10.7284 (19) Å
c = 22.705 (4) Å
β = 91.759 (3)°
V = 2430.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 295 (2) K
0.11 × 0.08 × 0.05 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.881, T_{max} = 0.943
17254 measured reflections
4754 independent reflections
3608 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.104
S = 1.04
4754 reflections
287 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Science Foundation of Shandong Province and Qufu Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ2007).

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supporting information

Acta Cryst. (2008). E**64**, m98 [https://doi.org/10.1107/S1600536807064471]

[*N*-(5-Chloro-2-oxidobenzylidene)valinato-κ^3O,N,O']dicyclohexyltin(IV)

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S1. Comment

The organotin complexes with Schiff bases derived from α-amino acids continue to receives attention due to their biological activities (Beltran *et al.*, 2003; Dakternieks *et al.*, 1998; Tian *et al.*, 2005, 2006, 2007). The structures of two dicyclohexyltin complexes with the Schiff base ligand, [*N*-(5-chloro-2-oxidophenylmethylene)isoleucinato]dicyclohexyltin (Tian *et al.*, 2004) and [*N*-(3,5-dibromo-2-oxidophenylmethylene)alaninato]dicyclohexyltin (Tian *et al.*, 2007) have been reported. As a continuation of these studies, the structure of the title compound, (I), is now described.

The coordination geometry about the tin atom in (I) is that of a distorted trigonal bipyramid with two cyclohexyl groups and the imino N1 atom occupying the equatorial positions and the axial positions being occupied by phenoxide O1 atom and a unidentate carboxylate O2 atom (Fig. 1). The bond length of Sn—O1 was shorter than that of Sn—O2 and the bond angle O1—Sn—O2 was 155.75 (12) °. The monodentate mode of coordination of carboxylate is reflected in the disparate C9—O2 and C9—O3 bond lengths of 1.282 (5) and 1.221 (6) Å, respectively. The distances of bonds around the tin atom were comparable to those observed in the dicyclohexyltin complexes mentioned above.

S2. Experimental

The title compound was synthesized by the reaction of dicyclohexyltin dichloride (0.71 g, 2 mmol) with potassium *N*-(5-chlorosalicylidene)valinate (0.59 g, 2 mmol) in the presence of Et_3N (0.20 g, 2 mmol) in 40 ml me thanol. The reaction mixture was refluxed for 3 h and filtered. The yellow solid obtained, (I), by removal of solvent under reduce pressure was recrystallized from dichloromethane-petroleum ether (60–90) (1:1, V/V) and crystals of (I) were obtained from chloroform-hexane (1:1, V/V) by slow evaporation at room temperature (yield 67%, m.p. 439–440 K).

S3. Refinement

One cyclohexyl group (C19–C24) is disordered over two positions. The site occupancy factors were refined with sum constrained to 1, converging to 0.708 (10) for atoms C19–C24 and 0.292 (10) for atoms C19′–C24′. For the cyclohexyl rings, the carbon-carbon distance was constrained to 1.52 (1) Å and 1,3-related distance to 2.50 (2) Å. The C19 and C19′ atoms were constrained to occupy the same position, and the temperature factors for each pair of atoms were set to equal. H atoms were placed at calculated positions and were included in the refinement in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic H atoms, C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for methyl H atoms, and C—H = 0.98 Å and U_{iso}(H) = 1.2Ueq(C) for methine H atoms.

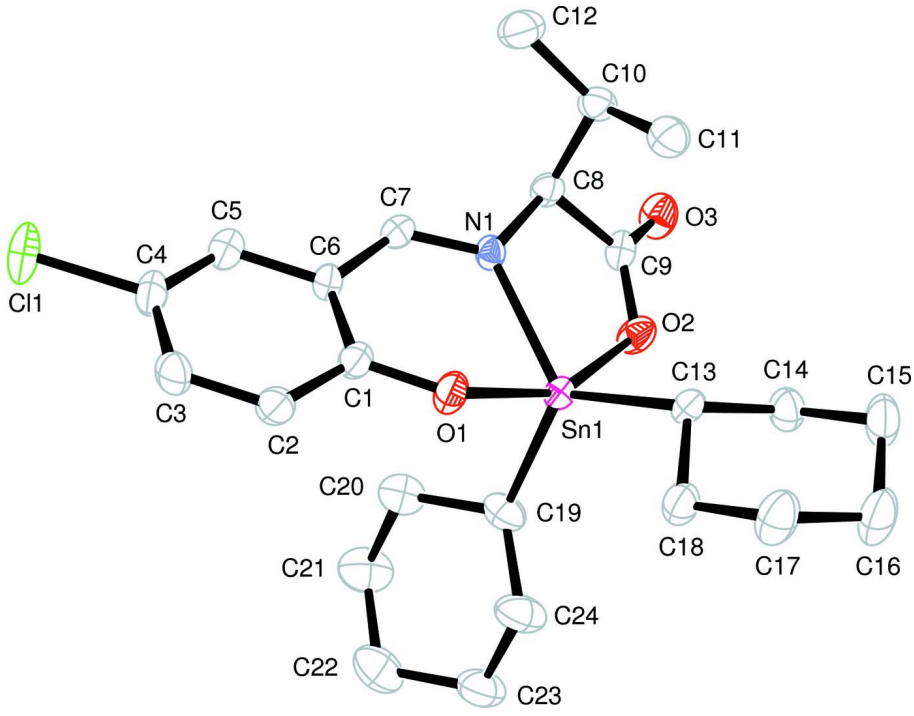

Figure 1

The structure of (I) with displacement ellipsoids are drawn at the 30% probability level. For cyclohexyl group C19–C24, the minor disordered component has been omitted for clarity.

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Crystal data

$[Sn(C_6H_{11})_2(C_{12}H_{12}ClNO_3)]$
$M_r = 538.66$
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Hall symbol: -P 2yn
$a = 9.9830\ (18)$ Å
$b = 10.7284\ (19)$ Å
$c = 22.705\ (4)$ Å
$\beta = 91.759\ (3)°$
$V = 2430.6\ (7)$ Å^3
$Z = 4$
$F(000) = 1104$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2430 reflections
$\theta = 2.6–19.8°$
$\mu = 1.19$ mm^{-1}
$T = 295$ K
Prism, yellow
0.11 × 0.08 × 0.05 mm

Data collection

Bruker SMART APEX detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.881$, $T_{max} = 0.943$
17254 measured reflections
4754 independent reflections
3608 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -12\rightarrow12$
$k = -13\rightarrow13$
$l = -27\rightarrow27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.104$
$S = 1.04$
4754 reflections
287 parameters
24 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
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.1331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.80$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	1.12598 (3)	0.20087 (3)	0.854731 (14)	0.03571 (12)	
N1	1.1870 (3)	0.3911 (3)	0.83569 (15)	0.0337 (8)	
O1	1.0335 (3)	0.2897 (3)	0.92506 (14)	0.0471 (8)	
O2	1.2493 (3)	0.1893 (3)	0.77824 (14)	0.0482 (8)	
O3	1.3868 (4)	0.2863 (3)	0.71861 (15)	0.0581 (10)	
Cl1	0.75627 (17)	0.76889 (14)	0.93223 (7)	0.0752 (5)	
C1	0.9725 (5)	0.3979 (4)	0.9241 (2)	0.0399 (11)	
C2	0.8670 (5)	0.4189 (4)	0.9628 (2)	0.0472 (12)	
H2	0.8410	0.3548	0.9875	0.057*	
C3	0.8021 (5)	0.5305 (5)	0.9648 (2)	0.0512 (13)	
H3	0.7324	0.5419	0.9905	0.061*	
C4	0.8407 (5)	0.6271 (4)	0.9284 (2)	0.0478 (13)	
C5	0.9418 (5)	0.6126 (4)	0.8906 (2)	0.0454 (12)	
H5	0.9671	0.6788	0.8669	0.054*	
C6	1.0087 (4)	0.4973 (4)	0.88714 (18)	0.0342 (10)	
C7	1.1167 (4)	0.4896 (4)	0.84753 (19)	0.0382 (11)	
H7	1.1392	0.5626	0.8281	0.046*	
C8	1.3004 (4)	0.4043 (4)	0.79714 (19)	0.0386 (11)	
H8	1.2814	0.4732	0.7699	0.046*	
C9	1.3146 (5)	0.2848 (4)	0.7611 (2)	0.0407 (11)	
C10	1.4318 (5)	0.4346 (4)	0.8325 (2)	0.0462 (12)	
H10	1.5042	0.4359	0.8043	0.055*	
C11	1.4686 (5)	0.3373 (5)	0.8786 (2)	0.0574 (14)	
H11A	1.4726	0.2567	0.8603	0.086*	
H11B	1.4022	0.3364	0.9083	0.086*	

H11C	1.5545	0.3571	0.8965	0.086*	
C12	1.4268 (5)	0.5636 (5)	0.8605 (2)	0.0634 (16)	
H12A	1.4041	0.6243	0.8308	0.095*	
H12B	1.5128	0.5833	0.8781	0.095*	
H12C	1.3604	0.5645	0.8902	0.095*	
C13	1.2432 (4)	0.0796 (4)	0.9097 (2)	0.0391 (11)	
H13	1.3021	0.1314	0.9349	0.047*	
C14	1.3322 (5)	−0.0079 (4)	0.8743 (2)	0.0499 (13)	
H14A	1.2764	−0.0575	0.8476	0.060*	
H14B	1.3925	0.0412	0.8510	0.060*	
C15	1.4130 (6)	−0.0934 (5)	0.9149 (3)	0.0662 (16)	
H15A	1.4647	−0.1505	0.8915	0.079*	
H15B	1.4754	−0.0440	0.9388	0.079*	
C16	1.3243 (6)	−0.1665 (5)	0.9545 (3)	0.0728 (18)	
H16A	1.3794	−0.2163	0.9814	0.087*	
H16B	1.2690	−0.2229	0.9308	0.087*	
C17	1.2343 (6)	−0.0816 (5)	0.9898 (2)	0.0666 (16)	
H17A	1.1739	−0.1319	1.0125	0.080*	
H17B	1.2889	−0.0323	1.0171	0.080*	
C18	1.1540 (5)	0.0037 (4)	0.9497 (2)	0.0502 (13)	
H18A	1.1019	0.0600	0.9733	0.060*	
H18B	1.0920	−0.0455	0.9256	0.060*	
C19	0.9504 (4)	0.1411 (5)	0.8079 (2)	0.0554 (14)	0.708 (10)
H19A	0.9779	0.0674	0.7858	0.066*	0.708 (10)
C20	0.8944 (8)	0.2290 (7)	0.7624 (4)	0.055 (2)	0.708 (10)
H20A	0.9633	0.2479	0.7346	0.066*	0.708 (10)
H20B	0.8700	0.3062	0.7815	0.066*	0.708 (10)
C21	0.7723 (9)	0.1776 (11)	0.7290 (4)	0.077 (3)	0.708 (10)
H21A	0.7344	0.2422	0.7037	0.092*	0.708 (10)
H21B	0.7996	0.1091	0.7042	0.092*	0.708 (10)
C22	0.6677 (9)	0.1328 (13)	0.7698 (6)	0.081 (3)	0.708 (10)
H22A	0.5976	0.0910	0.7468	0.098*	0.708 (10)
H22B	0.6279	0.2043	0.7886	0.098*	0.708 (10)
C23	0.7204 (8)	0.0447 (10)	0.8168 (4)	0.072 (3)	0.708 (10)
H23A	0.7417	−0.0346	0.7988	0.087*	0.708 (10)
H23B	0.6509	0.0301	0.8449	0.087*	0.708 (10)
C24	0.8441 (8)	0.0943 (10)	0.8492 (4)	0.071 (3)	0.708 (10)
H24A	0.8824	0.0287	0.8739	0.085*	0.708 (10)
H24B	0.8183	0.1621	0.8748	0.085*	0.708 (10)
C19′	0.9504 (4)	0.1411 (5)	0.8079 (2)	0.0554 (14)	0.292 (10)
H19B	0.9825	0.1101	0.7702	0.066*	0.292 (10)
C20′	0.8588 (15)	0.2491 (12)	0.7912 (9)	0.055 (2)	0.292 (10)
H20C	0.8289	0.2885	0.8270	0.066*	0.292 (10)
H20D	0.9096	0.3104	0.7698	0.066*	0.292 (10)
C21′	0.737 (2)	0.212 (2)	0.7539 (10)	0.077 (3)	0.292 (10)
H21C	0.6769	0.2824	0.7495	0.092*	0.292 (10)
H21D	0.7649	0.1876	0.7150	0.092*	0.292 (10)
C22′	0.6640 (17)	0.105 (2)	0.7817 (17)	0.081 (3)	0.292 (10)

H22C	0.6241	0.1332	0.8177	0.098*	0.292 (10)
H22D	0.5921	0.0771	0.7551	0.098*	0.292 (10)
C23′	0.7553 (19)	−0.0043 (17)	0.7958 (12)	0.072 (3)	0.292 (10)
H23C	0.7850	−0.0405	0.7593	0.087*	0.292 (10)
H23D	0.7055	−0.0675	0.8164	0.087*	0.292 (10)
C24′	0.8766 (18)	0.0332 (17)	0.8333 (10)	0.071 (3)	0.292 (10)
H24C	0.8479	0.0552	0.8724	0.085*	0.292 (10)
H24D	0.9369	−0.0374	0.8372	0.085*	0.292 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0373 (2)	0.02864 (17)	0.04125 (19)	0.00125 (14)	0.00194 (13)	−0.00021 (15)
N1	0.035 (2)	0.033 (2)	0.034 (2)	0.0053 (16)	0.0086 (16)	0.0009 (16)
O1	0.056 (2)	0.0334 (18)	0.053 (2)	0.0095 (15)	0.0164 (17)	0.0055 (15)
O2	0.063 (2)	0.0366 (19)	0.046 (2)	−0.0013 (16)	0.0115 (17)	−0.0090 (15)
O3	0.071 (3)	0.057 (2)	0.048 (2)	0.0110 (19)	0.0197 (19)	−0.0038 (18)
Cl1	0.0850 (11)	0.0588 (9)	0.0823 (11)	0.0411 (8)	0.0093 (9)	−0.0086 (8)
C1	0.043 (3)	0.034 (3)	0.043 (3)	0.002 (2)	−0.001 (2)	−0.003 (2)
C2	0.048 (3)	0.041 (3)	0.053 (3)	−0.003 (2)	0.018 (2)	−0.001 (2)
C3	0.045 (3)	0.055 (3)	0.055 (3)	0.005 (2)	0.012 (2)	−0.015 (3)
C4	0.048 (3)	0.042 (3)	0.052 (3)	0.016 (2)	−0.006 (3)	−0.007 (2)
C5	0.052 (3)	0.039 (3)	0.045 (3)	0.007 (2)	−0.002 (2)	−0.002 (2)
C6	0.038 (3)	0.031 (2)	0.034 (2)	0.0065 (19)	0.004 (2)	−0.0007 (19)
C7	0.043 (3)	0.029 (2)	0.042 (3)	0.000 (2)	0.001 (2)	0.002 (2)
C8	0.043 (3)	0.034 (2)	0.039 (3)	−0.001 (2)	0.009 (2)	0.005 (2)
C9	0.047 (3)	0.040 (3)	0.035 (3)	0.012 (2)	−0.001 (2)	−0.002 (2)
C10	0.041 (3)	0.044 (3)	0.054 (3)	−0.007 (2)	0.011 (2)	−0.005 (2)
C11	0.052 (3)	0.056 (3)	0.063 (4)	−0.002 (3)	−0.007 (3)	0.002 (3)
C12	0.067 (4)	0.050 (3)	0.073 (4)	−0.012 (3)	0.003 (3)	−0.009 (3)
C13	0.043 (3)	0.027 (2)	0.047 (3)	0.001 (2)	−0.001 (2)	0.001 (2)
C14	0.047 (3)	0.051 (3)	0.052 (3)	0.010 (2)	0.012 (2)	0.005 (2)
C15	0.059 (4)	0.059 (4)	0.082 (4)	0.026 (3)	0.015 (3)	0.008 (3)
C16	0.087 (5)	0.052 (3)	0.079 (4)	0.027 (3)	0.009 (4)	0.018 (3)
C17	0.085 (4)	0.054 (3)	0.062 (4)	0.016 (3)	0.014 (3)	0.014 (3)
C18	0.054 (3)	0.039 (3)	0.058 (3)	0.008 (2)	0.016 (3)	0.009 (2)
C19	0.040 (3)	0.063 (3)	0.063 (4)	−0.007 (3)	−0.006 (3)	−0.006 (3)
C20	0.059 (5)	0.072 (5)	0.033 (5)	−0.011 (4)	−0.009 (4)	0.005 (4)
C21	0.075 (6)	0.097 (8)	0.055 (7)	−0.017 (5)	−0.026 (5)	0.011 (5)
C22	0.049 (4)	0.109 (8)	0.086 (8)	−0.004 (4)	−0.016 (4)	0.002 (6)
C23	0.050 (5)	0.081 (8)	0.085 (8)	−0.019 (5)	−0.004 (5)	0.006 (5)
C24	0.050 (5)	0.086 (8)	0.076 (6)	−0.020 (5)	−0.015 (4)	0.028 (6)
C19′	0.040 (3)	0.063 (3)	0.063 (4)	−0.007 (3)	−0.006 (3)	−0.006 (3)
C20′	0.059 (5)	0.072 (5)	0.033 (5)	−0.011 (4)	−0.009 (4)	0.005 (4)
C21′	0.075 (6)	0.097 (8)	0.055 (7)	−0.017 (5)	−0.026 (5)	0.011 (5)
C22′	0.049 (4)	0.109 (8)	0.086 (8)	−0.004 (4)	−0.016 (4)	0.002 (6)
C23′	0.050 (5)	0.081 (8)	0.085 (8)	−0.019 (5)	−0.004 (5)	0.006 (5)
C24′	0.050 (5)	0.086 (8)	0.076 (6)	−0.020 (5)	−0.015 (4)	0.028 (6)

Geometric parameters (Å, º)

Sn1—O1	2.098 (3)	C15—H15A	0.9700
Sn1—C19	2.122 (4)	C15—H15B	0.9700
Sn1—C13	2.128 (4)	C16—C17	1.525 (7)
Sn1—O2	2.163 (3)	C16—H16A	0.9700
Sn1—N1	2.177 (4)	C16—H16B	0.9700
N1—C7	1.301 (5)	C17—C18	1.504 (6)
N1—C8	1.459 (5)	C17—H17A	0.9700
O1—C1	1.311 (5)	C17—H17B	0.9700
O2—C9	1.282 (5)	C18—H18A	0.9700
O3—C9	1.221 (6)	C18—H18B	0.9700
Cl1—C4	1.742 (5)	C19—C20	1.494 (7)
C1—C2	1.409 (6)	C19—C24	1.524 (7)
C1—C6	1.411 (6)	C19—H19A	0.9800
C2—C3	1.363 (6)	C20—C21	1.519 (7)
C2—H2	0.9300	C20—H20A	0.9700
C3—C4	1.387 (7)	C20—H20B	0.9700
C3—H3	0.9300	C21—C22	1.496 (8)
C4—C5	1.354 (6)	C21—H21A	0.9700
C5—C6	1.410 (6)	C21—H21B	0.9700
C5—H5	0.9300	C22—C23	1.509 (8)
C6—C7	1.428 (6)	C22—H22A	0.9700
C7—H7	0.9300	C22—H22B	0.9700
C8—C9	1.530 (6)	C23—C24	1.515 (7)
C8—C10	1.552 (6)	C23—H23A	0.9700
C8—H8	0.9800	C23—H23B	0.9700
C10—C11	1.516 (7)	C24—H24A	0.9700
C10—C12	1.525 (6)	C24—H24B	0.9700
C10—H10	0.9800	C20′—C21′	1.515 (9)
C11—H11A	0.9600	C20′—H20C	0.9700
C11—H11B	0.9600	C20′—H20D	0.9700
C11—H11C	0.9600	C21′—C22′	1.510 (10)
C12—H12A	0.9600	C21′—H21C	0.9700
C12—H12B	0.9600	C21′—H21D	0.9700
C12—H12C	0.9600	C22′—C23′	1.510 (10)
C13—C18	1.527 (6)	C22′—H22C	0.9700
C13—C14	1.535 (6)	C22′—H22D	0.9700
C13—H13	0.9800	C23′—C24′	1.513 (10)
C14—C15	1.516 (6)	C23′—H23C	0.9700
C14—H14A	0.9700	C23′—H23D	0.9700
C14—H14B	0.9700	C24′—H24C	0.9700
C15—C16	1.502 (7)	C24′—H24D	0.9700
O1—Sn1—C19	98.23 (17)	H15A—C15—H15B	108.0
O1—Sn1—C13	94.51 (15)	C15—C16—C17	111.7 (5)
C19—Sn1—C13	122.71 (18)	C15—C16—H16A	109.3
O1—Sn1—O2	155.75 (12)	C17—C16—H16A	109.3

C19—Sn1—O2	93.54 (17)	C15—C16—H16B	109.3
C13—Sn1—O2	96.83 (15)	C17—C16—H16B	109.3
O1—Sn1—N1	81.80 (12)	H16A—C16—H16B	107.9
C19—Sn1—N1	114.56 (16)	C18—C17—C16	110.9 (5)
C13—Sn1—N1	122.50 (15)	C18—C17—H17A	109.5
O2—Sn1—N1	74.02 (12)	C16—C17—H17A	109.5
C7—N1—C8	118.6 (4)	C18—C17—H17B	109.5
C7—N1—Sn1	124.3 (3)	C16—C17—H17B	109.5
C8—N1—Sn1	115.9 (3)	H17A—C17—H17B	108.1
C1—O1—Sn1	127.2 (3)	C17—C18—C13	112.0 (4)
C9—O2—Sn1	120.4 (3)	C17—C18—H18A	109.2
O1—C1—C2	119.1 (4)	C13—C18—H18A	109.2
O1—C1—C6	123.4 (4)	C17—C18—H18B	109.2
C2—C1—C6	117.4 (4)	C13—C18—H18B	109.2
C3—C2—C1	121.8 (5)	H18A—C18—H18B	107.9
C3—C2—H2	119.1	C20—C19—C24	112.4 (5)
C1—C2—H2	119.1	C20—C19—Sn1	116.2 (4)
C2—C3—C4	119.7 (5)	C24—C19—Sn1	111.7 (4)
C2—C3—H3	120.2	C20—C19—H19A	105.1
C4—C3—H3	120.2	C24—C19—H19A	105.1
C5—C4—C3	121.2 (4)	Sn1—C19—H19A	105.1
C5—C4—Cl1	120.2 (4)	C19—C20—C21	113.2 (6)
C3—C4—Cl1	118.6 (4)	C19—C20—H20A	108.9
C4—C5—C6	120.0 (5)	C21—C20—H20A	108.9
C4—C5—H5	120.0	C19—C20—H20B	108.9
C6—C5—H5	120.0	C21—C20—H20B	108.9
C5—C6—C1	120.0 (4)	H20A—C20—H20B	107.8
C5—C6—C7	117.0 (4)	C22—C21—C20	111.8 (7)
C1—C6—C7	122.9 (4)	C22—C21—H21A	109.2
N1—C7—C6	126.9 (4)	C20—C21—H21A	109.2
N1—C7—H7	116.6	C22—C21—H21B	109.2
C6—C7—H7	116.6	C20—C21—H21B	109.2
N1—C8—C9	109.1 (4)	H21A—C21—H21B	107.9
N1—C8—C10	111.7 (4)	C21—C22—C23	113.9 (7)
C9—C8—C10	111.2 (4)	C21—C22—H22A	108.8
N1—C8—H8	108.3	C23—C22—H22A	108.8
C9—C8—H8	108.3	C21—C22—H22B	108.8
C10—C8—H8	108.3	C23—C22—H22B	108.8
O3—C9—O2	124.6 (4)	H22A—C22—H22B	107.7
O3—C9—C8	118.6 (4)	C22—C23—C24	112.7 (7)
O2—C9—C8	116.8 (4)	C22—C23—H23A	109.1
C11—C10—C12	110.4 (4)	C24—C23—H23A	109.1
C11—C10—C8	113.4 (4)	C22—C23—H23B	109.1
C12—C10—C8	111.6 (4)	C24—C23—H23B	109.1
C11—C10—H10	107.1	H23A—C23—H23B	107.8
C12—C10—H10	107.1	C23—C24—C19	112.9 (6)
C8—C10—H10	107.1	C23—C24—H24A	109.0
C10—C11—H11A	109.5	C19—C24—H24A	109.0

C10—C11—H11B	109.5	C23—C24—H24B	109.0
H11A—C11—H11B	109.5	C19—C24—H24B	109.0
C10—C11—H11C	109.5	H24A—C24—H24B	107.8
H11A—C11—H11C	109.5	C21′—C20′—H20C	108.8
H11B—C11—H11C	109.5	C21′—C20′—H20D	108.8
C10—C12—H12A	109.5	H20C—C20′—H20D	107.7
C10—C12—H12B	109.5	C22′—C21′—C20′	110.9 (12)
H12A—C12—H12B	109.5	C22′—C21′—H21C	109.5
C10—C12—H12C	109.5	C20′—C21′—H21C	109.5
H12A—C12—H12C	109.5	C22′—C21′—H21D	109.5
H12B—C12—H12C	109.5	C20′—C21′—H21D	109.5
C18—C13—C14	110.0 (4)	H21C—C21′—H21D	108.0
C18—C13—Sn1	110.8 (3)	C23′—C22′—C21′	112.4 (14)
C14—C13—Sn1	112.6 (3)	C23′—C22′—H22C	109.1
C18—C13—H13	107.8	C21′—C22′—H22C	109.1
C14—C13—H13	107.8	C23′—C22′—H22D	109.1
Sn1—C13—H13	107.8	C21′—C22′—H22D	109.1
C15—C14—C13	111.0 (4)	H22C—C22′—H22D	107.9
C15—C14—H14A	109.4	C22′—C23′—C24′	112.4 (13)
C13—C14—H14A	109.4	C22′—C23′—H23C	109.1
C15—C14—H14B	109.4	C24′—C23′—H23C	109.1
C13—C14—H14B	109.4	C22′—C23′—H23D	109.1
H14A—C14—H14B	108.0	C24′—C23′—H23D	109.1
C16—C15—C14	111.5 (4)	H23C—C23′—H23D	107.8
C16—C15—H15A	109.3	C23′—C24′—H24C	109.1
C14—C15—H15A	109.3	C23′—C24′—H24D	109.1
C16—C15—H15B	109.3	H24C—C24′—H24D	107.8
C14—C15—H15B	109.3		

O1—Sn1—N1—C7	−31.2 (3)	C10—C8—C9—O3	−70.2 (5)
C19—Sn1—N1—C7	64.1 (4)	N1—C8—C9—O2	−14.2 (5)
C13—Sn1—N1—C7	−121.4 (3)	C10—C8—C9—O2	109.4 (5)
O2—Sn1—N1—C7	150.7 (4)	N1—C8—C10—C11	58.1 (5)
O1—Sn1—N1—C8	161.1 (3)	C9—C8—C10—C11	−64.0 (5)
C19—Sn1—N1—C8	−103.5 (3)	N1—C8—C10—C12	−67.3 (5)
C13—Sn1—N1—C8	71.0 (3)	C9—C8—C10—C12	170.6 (4)
O2—Sn1—N1—C8	−17.0 (3)	O1—Sn1—C13—C18	56.4 (3)
C19—Sn1—O1—C1	−75.0 (4)	C19—Sn1—C13—C18	−46.4 (4)
C13—Sn1—O1—C1	161.0 (4)	O2—Sn1—C13—C18	−145.1 (3)
O2—Sn1—O1—C1	43.2 (6)	N1—Sn1—C13—C18	139.5 (3)
N1—Sn1—O1—C1	38.8 (4)	O1—Sn1—C13—C14	180.0 (3)
O1—Sn1—O2—C9	4.6 (5)	C19—Sn1—C13—C14	77.2 (4)
C19—Sn1—O2—C9	123.7 (4)	O2—Sn1—C13—C14	−21.5 (3)
C13—Sn1—O2—C9	−112.7 (3)	N1—Sn1—C13—C14	−96.9 (3)
N1—Sn1—O2—C9	9.2 (3)	C18—C13—C14—C15	−55.4 (5)
Sn1—O1—C1—C2	150.7 (3)	Sn1—C13—C14—C15	−179.5 (4)
Sn1—O1—C1—C6	−30.9 (6)	C13—C14—C15—C16	56.0 (6)
O1—C1—C2—C3	178.3 (4)	C14—C15—C16—C17	−55.6 (7)

C6—C1—C2—C3	−0.2 (7)	C15—C16—C17—C18	54.9 (7)
C1—C2—C3—C4	−0.5 (8)	C16—C17—C18—C13	−55.4 (6)
C2—C3—C4—C5	0.1 (8)	C14—C13—C18—C17	55.8 (6)
C2—C3—C4—Cl1	−179.8 (4)	Sn1—C13—C18—C17	−179.1 (4)
C3—C4—C5—C6	0.8 (7)	O1—Sn1—C19—C20	90.7 (5)
Cl1—C4—C5—C6	−179.2 (4)	C13—Sn1—C19—C20	−168.5 (5)
C4—C5—C6—C1	−1.5 (7)	O2—Sn1—C19—C20	−68.0 (5)
C4—C5—C6—C7	−178.3 (4)	N1—Sn1—C19—C20	6.0 (6)
O1—C1—C6—C5	−177.2 (4)	O1—Sn1—C19—C24	−40.1 (6)
C2—C1—C6—C5	1.2 (6)	C13—Sn1—C19—C24	60.7 (6)
O1—C1—C6—C7	−0.6 (7)	O2—Sn1—C19—C24	161.2 (6)
C2—C1—C6—C7	177.8 (4)	N1—Sn1—C19—C24	−124.8 (6)
C8—N1—C7—C6	−175.4 (4)	C24—C19—C20—C21	−51.9 (9)
Sn1—N1—C7—C6	17.3 (6)	Sn1—C19—C20—C21	177.6 (5)
C5—C6—C7—N1	−176.5 (4)	C19—C20—C21—C22	52.2 (11)
C1—C6—C7—N1	6.8 (7)	C20—C21—C22—C23	−51.0 (14)
C7—N1—C8—C9	−146.8 (4)	C21—C22—C23—C24	50.0 (14)
Sn1—N1—C8—C9	21.6 (4)	C22—C23—C24—C19	−48.9 (11)
C7—N1—C8—C10	89.9 (5)	C20—C19—C24—C23	50.3 (9)
Sn1—N1—C8—C10	−101.7 (3)	Sn1—C19—C24—C23	−177.0 (6)
Sn1—O2—C9—O3	179.7 (4)	C20′—C21′—C22′—C23′	−53 (3)
Sn1—O2—C9—C8	0.1 (5)	C21′—C22′—C23′—C24′	54 (3)
N1—C8—C9—O3	166.2 (4)		