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

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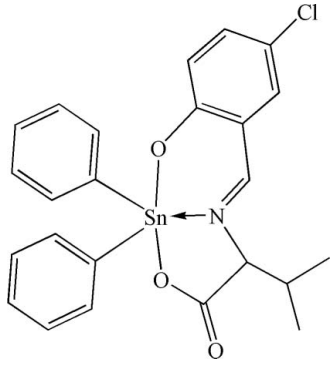
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.031; wR factor = 0.067; data-to-parameter ratio = 15.9.

The Sn atom of the title compound, $[Sn(C_6H_5)_2(C_{12}H_{12}ClNO_3)]$, is in a distorted $SnNC_2O_2$ trigonal–bipyramidal geometry and forms five- and six-membered chelate rings with the tridentate ligand. One phenyl group is disordered over two positions with occupancy factors 0.58 (3):0.42 (3).

Related literature

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



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_{12}H_{12}ClNO_3)]$
M_r = 526.57
Monoclinic, $P2_1$
a = 9.5105 (11) Å
b = 11.3594 (13) Å
c = 10.4939 (12) Å
β = 91.305 (2)°
V = 1133.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.27 mm^{-1}
T = 295 (2) K
0.13 × 0.10 × 0.07 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.852, T_{max} = 0.916
9180 measured reflections
4590 independent reflections
4284 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.067
S = 1.02
4590 reflections
289 parameters
19 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Absolute structure: Flack (1983), with 2135 Friedel pairs
Flack parameter: 0.03 (2)

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2308).

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supplementary materials

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

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Comment

The structural chemistry of diorganotin complexes with Schiff bases derived from α-amino acids receives attention since their antitumour activities and the quadratic nonlinear optical properties (Beltran *et al.*, 2003; Dakternieks *et al.*, 1998; Tian *et al.*, 2005, 2006, 2007; Rivera *et al.*, 2006). The structures of several diorganotin complexes with the Schiff base ligand, [*N*-(2-oxidohydroxyphenylmethylene)valine, such as [*N*-(2-oxidophenylmethylene)valinato]dibutyltin(IV), [*N*-(2-oxidophenylmethylene)valinato]diphenyltin(IV) (Beltran *et al.*, 2003), [*N*-(4-diethylamino-2-oxidophenylmethylene)valinato]diphenyltin(IV) (Rivera *et al.*, 2006), [*N*-(2-oxidophenylmethylene)valinato]di-t-butyltin(IV) (Ding *et al.*, 2006), [*N*-(5-bromo-2-oxidophenylmethylene)valinato]diphenyltin(IV), [*N*-(3,5-dibromo-2-oxidophenylmethylene)valinato]diphenyltin(IV) and [*N*-(3,5-dibromo-2-oxidophenylmethylene)valinato]dibutyltin(IV) (Tian *et al.*, 2005, 2006, 2007) have been reported.

The coordination geometry about the tin atom in the title compound, (I), is that of a distorted trigonal bipyramid with two phenyl groups and the imino N1 atom occupying the equatorial positions and the axial positions being occupied by a unidentate carboxylate O1 atom and phenoxide O2 atom (Fig. 1). The bond length of Sn—O2 was longer than that of Sn—O1 and the bond angle O1—Sn—O2 was 157.87 (11)°. The monodentate mode of coordination of carboxylate is reflected in the disparate C9—O2 and C9—O3 bond lengths of 1.290 (6) and 1.200 (6) Å, respectively. The distances of bonds around the tin atom were comparable to those observed in the diphenyltin complexes mentioned above.

Experimental

The title compound was synthesized by the reaction of diphenyltin dichloride (0.69 g, 2 mmol) with potassium *N*-(5-chlorosalicylidene)-(*L*)-valinate (0.59 g, 2 mmol) in the presence of Et_3N (0.20 g, 2 mmol) in 60 ml benzene. 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) (1:2, V/V) and crystals of (I) were obtained from chloroform-hexane (1:1, V/V) by slow evaporation at temperature (yield 61%, m.p. 523–524 K).

Refinement

One phenyl group (C19–C24) is disordered over two positions; *ipso* atom C19 was refined with full occupancy, while the other atoms were refined in two parts, with site occupancy factors of 0.58 (3) (atoms C20–C24) and 0.42 (3) (atoms C20'–C24'). The phenyl rings were restrained to be planar regular hexagons, with target C⋯C distances of 1.39 (1) Å. The absolute configuration of the compound (I) was assigned on the basis of the known configuration of the starting reagent, (*L*)-valine. 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.

Figures

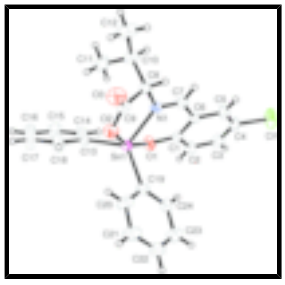


Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. For phenyl group C19–C14, the minor disordered component has been omitted for clarity.

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

Crystal data

$[Sn(C_6H_5)_2(C_{12}H_{12}ClNO_3)]$	F_{000} = 528
M_r = 526.57	D_x = 1.543 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3681 reflections
a = 9.5105 (11) Å	θ = 2.6–23.6º
b = 11.3594 (13) Å	μ = 1.27 mm^{-1}
c = 10.4939 (12) Å	T = 295 (2) K
β = 91.305 (2)º	Block, yellow
V = 1133.4 (2) Å^3	0.13 × 0.10 × 0.07 mm
Z = 2	

Data collection

Bruker SMART APEX area-detector diffractometer	4590 independent reflections
Radiation source: fine-focus sealed tube	4284 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 295(2) K	θ_{max} = 26.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −11→11
T_{min} = 0.852, T_{max} = 0.916	k = −14→14
9180 measured reflections	l = −12→13

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.067$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.40$ e Å^{-3}
4590 reflections	$\Delta\rho_{min} = -0.45$ e Å^{-3}
289 parameters	Extinction correction: none
19 restraints	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.03 (2)
Secondary atom site location: difference Fourier map	

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}	Occ. (<1)
Sn1	0.70895 (2)	0.99509 (4)	0.831297 (19)	0.03600 (8)	
Cl1	1.13466 (16)	0.52770 (11)	0.54971 (14)	0.0832 (5)	
O1	0.8224 (3)	0.8460 (3)	0.8791 (3)	0.0450 (7)	
O2	0.5607 (3)	1.1018 (3)	0.7298 (3)	0.0493 (7)	
O3	0.4190 (4)	1.1202 (3)	0.5617 (4)	0.0694 (11)	
N1	0.6499 (3)	0.8924 (3)	0.6661 (3)	0.0338 (7)	
C1	0.8890 (4)	0.7729 (4)	0.8023 (5)	0.0398 (11)	
C2	1.0045 (4)	0.7085 (4)	0.8506 (4)	0.0466 (10)	
H2	1.0327	0.7175	0.9355	0.056*	
C3	1.0755 (5)	0.6330 (4)	0.7744 (5)	0.0545 (12)	
H3	1.1514	0.5905	0.8077	0.065*	
C4	1.0353 (5)	0.6191 (4)	0.6476 (4)	0.0494 (11)	
C5	0.9224 (5)	0.6768 (4)	0.5986 (4)	0.0471 (10)	
H5	0.8946	0.6643	0.5141	0.056*	
C6	0.8465 (4)	0.7554 (3)	0.6741 (4)	0.0362 (8)	
C7	0.7225 (4)	0.8101 (3)	0.6175 (4)	0.0389 (9)	
H7	0.6929	0.7825	0.5379	0.047*	
C8	0.5227 (5)	0.9352 (5)	0.5940 (5)	0.0399 (12)	
H8	0.5401	0.9296	0.5025	0.048*	
C9	0.4979 (5)	1.0633 (4)	0.6278 (5)	0.0426 (13)	
C10	0.3968 (5)	0.8528 (5)	0.6264 (5)	0.0549 (13)	
H10	0.4284	0.7716	0.6135	0.066*	
C11	0.3545 (5)	0.8629 (5)	0.7628 (5)	0.0758 (16)	
H11A	0.3239	0.9419	0.7793	0.114*	

H11B	0.4334	0.8443	0.8178	0.114*	
H11C	0.2791	0.8091	0.7786	0.114*	
C12	0.2732 (6)	0.8735 (6)	0.5346 (6)	0.101 (2)	
H12A	0.2016	0.8159	0.5492	0.151*	
H12B	0.3044	0.8670	0.4485	0.151*	
H12C	0.2357	0.9509	0.5480	0.151*	
C13	0.5895 (3)	0.9951 (6)	0.9989 (3)	0.0409 (7)	
C14	0.5991 (5)	0.9052 (4)	1.0871 (4)	0.0499 (11)	
H14	0.6574	0.8413	1.0718	0.060*	
C15	0.5231 (6)	0.9088 (5)	1.1980 (5)	0.0666 (14)	
H15	0.5311	0.8483	1.2575	0.080*	
C16	0.4367 (5)	1.0019 (8)	1.2188 (4)	0.0779 (14)	
H16	0.3838	1.0041	1.2921	0.094*	
C17	0.4268 (7)	1.0916 (6)	1.1336 (6)	0.090 (2)	
H17	0.3683	1.1553	1.1494	0.108*	
C18	0.5042 (6)	1.0885 (5)	1.0227 (5)	0.0669 (14)	
H18	0.4976	1.1502	0.9647	0.080*	
C19	0.8775 (4)	1.1131 (4)	0.8039 (4)	0.0468 (10)	
C20	0.849 (3)	1.2326 (8)	0.7949 (19)	0.065 (4)	0.58 (3)
H20	0.7547	1.2552	0.7978	0.077*	0.58 (3)
C21	0.948 (3)	1.321 (2)	0.782 (2)	0.089 (6)	0.58 (3)
H21	0.9219	1.4001	0.7803	0.107*	0.58 (3)
C22	1.086 (3)	1.288 (2)	0.771 (3)	0.079 (6)	0.58 (3)
H22	1.1558	1.3438	0.7581	0.094*	0.58 (3)
C23	1.121 (2)	1.1703 (19)	0.7802 (19)	0.062 (4)	0.58 (3)
H23	1.2145	1.1477	0.7730	0.074*	0.58 (3)
C24	1.0194 (9)	1.085 (2)	0.800 (2)	0.056 (4)	0.58 (3)
H24	1.0471	1.0071	0.8105	0.067*	0.58 (3)
C20'	0.846 (4)	1.2225 (12)	0.751 (2)	0.065 (4)	0.42 (3)
H20'	0.7541	1.2456	0.7301	0.077*	0.42 (3)
C21'	0.961 (4)	1.294 (3)	0.733 (3)	0.089 (6)	0.42 (3)
H21'	0.9491	1.3706	0.7025	0.107*	0.42 (3)
C22'	1.095 (5)	1.252 (4)	0.760 (4)	0.079 (6)	0.42 (3)
H22'	1.1710	1.2991	0.7373	0.094*	0.42 (3)
C23'	1.124 (3)	1.146 (3)	0.818 (3)	0.062 (4)	0.42 (3)
H23'	1.2152	1.1251	0.8441	0.074*	0.42 (3)
C24'	1.0109 (14)	1.071 (3)	0.836 (3)	0.056 (4)	0.42 (3)
H24'	1.0238	0.9957	0.8681	0.067*	0.42 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03674 (12)	0.03590 (12)	0.03530 (12)	0.00080 (17)	−0.00019 (8)	−0.00332 (18)
Cl1	0.1032 (10)	0.0702 (12)	0.0778 (8)	0.0400 (8)	0.0352 (7)	−0.0003 (6)
O1	0.0523 (17)	0.0489 (17)	0.0337 (15)	0.0148 (14)	−0.0012 (13)	−0.0038 (13)
O2	0.0505 (17)	0.0423 (16)	0.0547 (19)	0.0069 (13)	−0.0089 (15)	0.0054 (14)
O3	0.068 (2)	0.062 (2)	0.076 (3)	0.0115 (19)	−0.021 (2)	0.018 (2)
N1	0.0320 (17)	0.0361 (17)	0.0331 (17)	−0.0016 (14)	−0.0021 (14)	0.0023 (14)

C1	0.033 (2)	0.040 (2)	0.046 (3)	−0.0046 (19)	0.0032 (19)	0.0066 (19)
C2	0.047 (2)	0.048 (2)	0.045 (2)	0.004 (2)	−0.004 (2)	0.004 (2)
C3	0.049 (3)	0.046 (3)	0.069 (3)	0.011 (2)	0.011 (2)	0.010 (3)
C4	0.052 (3)	0.035 (2)	0.062 (3)	0.0059 (19)	0.021 (2)	−0.002 (2)
C5	0.058 (3)	0.041 (2)	0.043 (2)	0.003 (2)	0.010 (2)	−0.0047 (18)
C6	0.036 (2)	0.032 (2)	0.041 (2)	−0.0061 (16)	0.0053 (16)	−0.0026 (17)
C7	0.043 (2)	0.040 (2)	0.033 (2)	−0.0080 (18)	−0.0002 (16)	−0.0005 (17)
C8	0.029 (2)	0.055 (3)	0.035 (2)	−0.0020 (19)	−0.0040 (18)	0.009 (2)
C9	0.045 (3)	0.044 (3)	0.039 (3)	0.004 (2)	0.003 (2)	0.013 (2)
C10	0.036 (2)	0.063 (3)	0.065 (3)	−0.012 (2)	−0.011 (2)	0.007 (3)
C11	0.055 (3)	0.090 (4)	0.083 (4)	−0.025 (3)	0.015 (3)	0.008 (3)
C12	0.060 (4)	0.121 (6)	0.119 (5)	−0.040 (4)	−0.042 (4)	0.039 (4)
C13	0.0453 (18)	0.0398 (17)	0.0377 (16)	−0.001 (3)	0.0021 (13)	−0.007 (3)
C14	0.053 (3)	0.053 (3)	0.044 (2)	0.007 (2)	0.001 (2)	−0.004 (2)
C15	0.076 (4)	0.073 (4)	0.051 (3)	0.001 (3)	0.011 (3)	0.014 (3)
C16	0.082 (3)	0.095 (4)	0.058 (3)	0.010 (5)	0.031 (2)	−0.003 (5)
C17	0.100 (5)	0.093 (5)	0.079 (4)	0.043 (4)	0.042 (4)	0.001 (4)
C18	0.085 (4)	0.057 (3)	0.060 (3)	0.028 (3)	0.023 (3)	0.008 (2)
C19	0.048 (3)	0.054 (3)	0.038 (2)	−0.017 (2)	−0.0024 (19)	−0.004 (2)
C20	0.052 (4)	0.067 (4)	0.073 (11)	−0.025 (4)	−0.029 (8)	0.019 (5)
C21	0.091 (7)	0.062 (11)	0.115 (17)	−0.037 (8)	−0.033 (11)	0.018 (9)
C22	0.076 (6)	0.080 (15)	0.079 (7)	−0.042 (10)	−0.015 (5)	0.014 (11)
C23	0.054 (4)	0.083 (11)	0.049 (11)	−0.015 (5)	0.006 (7)	0.015 (7)
C24	0.049 (3)	0.057 (6)	0.063 (12)	−0.008 (3)	0.013 (4)	−0.008 (6)
C20'	0.052 (4)	0.067 (4)	0.073 (11)	−0.025 (4)	−0.029 (8)	0.019 (5)
C21'	0.091 (7)	0.062 (11)	0.115 (17)	−0.037 (8)	−0.033 (11)	0.018 (9)
C22'	0.076 (6)	0.080 (15)	0.079 (7)	−0.042 (10)	−0.015 (5)	0.014 (11)
C23'	0.054 (4)	0.083 (11)	0.049 (11)	−0.015 (5)	0.006 (7)	0.015 (7)
C24'	0.049 (3)	0.057 (6)	0.063 (12)	−0.008 (3)	0.013 (4)	−0.008 (6)

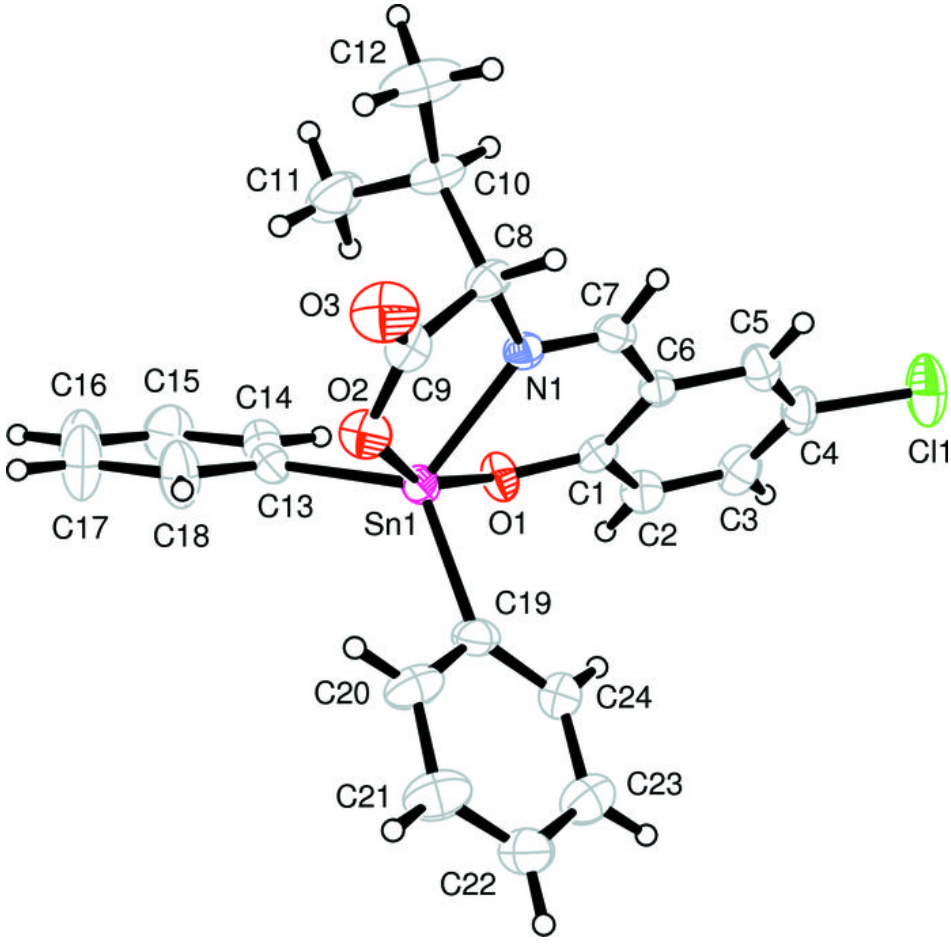
Geometric parameters (Å, °)

Sn1—O1	2.064 (3)	C13—C18	1.362 (7)
Sn1—C19	2.114 (4)	C13—C14	1.379 (7)
Sn1—C13	2.115 (3)	C14—C15	1.384 (6)
Sn1—O2	2.127 (3)	C14—H14	0.9300
Sn1—N1	2.153 (3)	C15—C16	1.360 (9)
Cl1—C4	1.753 (4)	C15—H15	0.9300
O1—C1	1.327 (5)	C16—C17	1.357 (9)
O2—C9	1.290 (6)	C16—H16	0.9300
O3—C9	1.200 (6)	C17—C18	1.392 (7)
N1—C7	1.276 (5)	C17—H17	0.9300
N1—C8	1.494 (5)	C18—H18	0.9300
C1—C2	1.405 (6)	C19—C20	1.388 (8)
C1—C6	1.410 (6)	C19—C24	1.388 (8)
C2—C3	1.363 (6)	C19—C24'	1.389 (9)
C2—H2	0.9300	C19—C20'	1.391 (9)
C3—C4	1.385 (7)	C20—C21	1.389 (8)
C3—H3	0.9300	C20—H20	0.9300

C4—C5	1.350 (6)	C21—C22	1.379 (9)
C5—C6	1.405 (6)	C21—H21	0.9300
C5—H5	0.9300	C22—C23	1.375 (9)
C6—C7	1.449 (6)	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.387 (8)
C8—C9	1.517 (6)	C23—H23	0.9300
C8—C10	1.564 (6)	C24—H24	0.9300
C8—H8	0.9800	C20'—C21'	1.389 (10)
C10—C11	1.500 (7)	C20'—H20'	0.9300
C10—C12	1.521 (7)	C21'—C22'	1.383 (10)
C10—H10	0.9800	C21'—H21'	0.9300
C11—H11A	0.9600	C22'—C23'	1.380 (10)
C11—H11B	0.9600	C22'—H22'	0.9300
C11—H11C	0.9600	C23'—C24'	1.387 (9)
C12—H12A	0.9600	C23'—H23'	0.9300
C12—H12B	0.9600	C24'—H24'	0.9300
C12—H12C	0.9600		
O1—Sn1—C19	99.17 (14)	C10—C12—H12C	109.5
O1—Sn1—C13	94.91 (19)	H12A—C12—H12C	109.5
C19—Sn1—C13	122.44 (19)	H12B—C12—H12C	109.5
O1—Sn1—O2	157.87 (11)	C18—C13—C14	118.9 (4)
C19—Sn1—O2	93.82 (14)	C18—C13—Sn1	119.1 (4)
C13—Sn1—O2	93.10 (16)	C14—C13—Sn1	122.0 (4)
O1—Sn1—N1	82.92 (11)	C13—C14—C15	121.0 (4)
C19—Sn1—N1	114.73 (14)	C13—C14—H14	119.5
C13—Sn1—N1	122.29 (16)	C15—C14—H14	119.5
O2—Sn1—N1	75.37 (11)	C16—C15—C14	119.1 (5)
C1—O1—Sn1	128.3 (3)	C16—C15—H15	120.5
C9—O2—Sn1	120.8 (3)	C14—C15—H15	120.5
C7—N1—C8	118.4 (3)	C17—C16—C15	120.8 (4)
C7—N1—Sn1	125.8 (3)	C17—C16—H16	119.6
C8—N1—Sn1	115.2 (3)	C15—C16—H16	119.6
O1—C1—C2	119.1 (4)	C16—C17—C18	120.1 (5)
O1—C1—C6	122.5 (4)	C16—C17—H17	120.0
C2—C1—C6	118.4 (4)	C18—C17—H17	120.0
C3—C2—C1	120.7 (4)	C13—C18—C17	120.1 (5)
C3—C2—H2	119.7	C13—C18—H18	119.9
C1—C2—H2	119.7	C17—C18—H18	119.9
C2—C3—C4	120.4 (4)	C20—C19—C24	114.5 (15)
C2—C3—H3	119.8	C20—C19—C24'	122.0 (18)
C4—C3—H3	119.8	C24—C19—C20'	113.4 (17)
C5—C4—C3	120.7 (4)	C24'—C19—C20'	126 (2)
C5—C4—Cl1	119.9 (4)	C20—C19—Sn1	118.6 (11)
C3—C4—Cl1	119.3 (4)	C24—C19—Sn1	126.8 (10)
C4—C5—C6	120.5 (4)	C24'—C19—Sn1	116.2 (13)
C4—C5—H5	119.7	C20'—C19—Sn1	117.4 (15)
C6—C5—H5	119.7	C19—C20—C21	125 (2)
C5—C6—C1	119.2 (4)	C19—C20—H20	117.3
C5—C6—C7	117.7 (4)	C21—C20—H20	117.3

C1—C6—C7	122.9 (4)	C22—C21—C20	117 (3)
N1—C7—C6	126.4 (4)	C22—C21—H21	121.3
N1—C7—H7	116.8	C20—C21—H21	121.3
C6—C7—H7	116.8	C23—C22—C21	119 (3)
N1—C8—C9	108.8 (4)	C23—C22—H22	120.4
N1—C8—C10	108.1 (4)	C21—C22—H22	120.4
C9—C8—C10	113.6 (4)	C22—C23—C24	121 (2)
N1—C8—H8	108.8	C22—C23—H23	119.3
C9—C8—H8	108.8	C24—C23—H23	119.3
C10—C8—H8	108.8	C23—C24—C19	121.7 (18)
O3—C9—O2	124.7 (5)	C23—C24—H24	119.2
O3—C9—C8	118.7 (5)	C19—C24—H24	119.2
O2—C9—C8	116.6 (5)	C21'—C20'—C19	114 (3)
C11—C10—C12	111.9 (5)	C21'—C20'—H20'	122.8
C11—C10—C8	112.6 (4)	C19—C20'—H20'	122.8
C12—C10—C8	110.7 (4)	C22'—C21'—C20'	120 (4)
C11—C10—H10	107.1	C22'—C21'—H21'	120.0
C12—C10—H10	107.1	C20'—C21'—H21'	120.0
C8—C10—H10	107.1	C23'—C22'—C21'	125 (4)
C10—C11—H11A	109.5	C23'—C22'—H22'	117.7
C10—C11—H11B	109.5	C21'—C22'—H22'	117.7
H11A—C11—H11B	109.5	C22'—C23'—C24'	116 (3)
C10—C11—H11C	109.5	C22'—C23'—H23'	121.8
H11A—C11—H11C	109.5	C24'—C23'—H23'	121.8
H11B—C11—H11C	109.5	C23'—C24'—C19	118 (2)
C10—C12—H12A	109.5	C23'—C24'—H24'	121.1
C10—C12—H12B	109.5	C19—C24'—H24'	121.1
H12A—C12—H12B	109.5		

Fig. 1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