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[*N*-(3,5-Dibromo-2-oxidobenzylidene)phenylalaninato-κ^3O,N,O']diphenyltin(IV)

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Key indicators

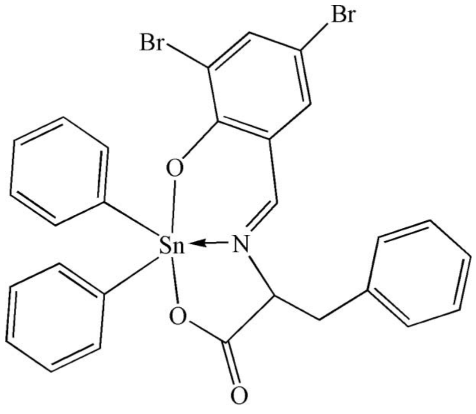
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.078
Data-to-parameter ratio = 17.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The Sn atom of the title compound, $[Sn(C_6H_5)_2(C_{16}H_{11}Br_2NO_3)]$, adopts a distorted $SnNC_2O_2$ trigonal–bipyramidal geometry and forms five- and six-membered chelate rings with the tridentate ligand.

Comment

The structural chemistry of diorganotin complexes with Schiff bases derived from α-amino acids continues to receive attention owing to their biological properties, especially their antitumour activities (Beltran *et al.*, 2003; Dakternieks *et al.*, 1998; Tian *et al.*, 2005, Tian *et al.*, 2006, 2007; Yin *et al.*, 2004). As a continuation of these studies, the synthesis and structure of the title compound, (I), are now described.



(I)

The coordination geometry about the tin atom in (I) is distorted trigonal bipyramidal, with two phenyl group C atoms (C17 and C23) and the imino N1 atom occupying the equatorial positions. The axial positions are occupied by the unidentate carboxylate atom O1 and the phenoxide atom O2 (Fig. 1). The Sn—O2 bond length is significantly longer than Sn—O1, and the O1—Sn—O2 angle is 157.50 (8)° (Table 1). The monodentate coordination mode of the carboxylate group is reflected in the disparate C9—O2 and C9—O3 bond lengths of 1.292 (4) and 1.212 (4) Å, respectively. Otherwise, the geometrical parameters for (I) are comparable to those observed in the diphenyltin complexes referenced above.

Experimental

The title compound was synthesized by the reaction of diphenyltin(IV) dichloride (0.69 g, 2 mmol) with potassium *N*-(3,5-dibromosalicylidene)phenylalaninate (0.93 g, 2 mmol), derived from potassium hydroxide, L-phenylalanine and 3,5-dibromosalicylaldehyde **[amounts of the three reagents?]** in the presence of Et_3N (0.20 g, 2 mmol) in methanol (60 ml). The reaction mixture was refluxed for 3 h, and then cooled to room temperature and filtered. The yellow solid obtained by removal of solvent under reduced pressure was recrystallized from ethanol and yellow plates of (I) were obtained by slow evaporation from chloroform–hexane (1:1 *v*/*v*) at 298 K (yield 67%; m.p. 393–394 K). Analysis found: C 48.31, H 3.00, N 2.03%; calculated for $C_{28}H_{21}Br_2NO_3Sn$: C 48.18, H 3.03, N 2.01%.

Crystal data

$[Sn(C_6H_5)_2(C_{16}H_{11}Br_2NO_3)]$
$M_r = 697.97$
Monoclinic, $P2_1/c$
$a = 11.2880\ (7)$ Å
$b = 23.3977\ (15)$ Å
$c = 10.7391\ (7)$ Å
$\beta = 113.074\ (1)^\circ$
$V = 2609.4\ (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 4.07$ mm^{-1}
$T = 295\ (2)$ K
$0.35 \times 0.25 \times 0.08$ mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.330$, $T_{max} = 0.737$
20999 measured reflections
5406 independent reflections
4566 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.078$
$S = 1.04$
5406 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.095 (2)	Sn1—O2	2.114 (2)
Sn1—C17	2.107 (3)	Sn1—N1	2.168 (2)
Sn1—C23	2.110 (3)		
O1—Sn1—C17	93.28 (10)	C23—Sn1—O2	96.06 (11)
O1—Sn1—C23	97.24 (10)	O1—Sn1—N1	82.35 (8)
C17—Sn1—C23	121.98 (11)	C17—Sn1—N1	122.87 (10)
O1—Sn1—O2	157.50 (8)	C23—Sn1—N1	115.06 (10)
C17—Sn1—O2	94.95 (11)	O2—Sn1—N1	75.59 (8)

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

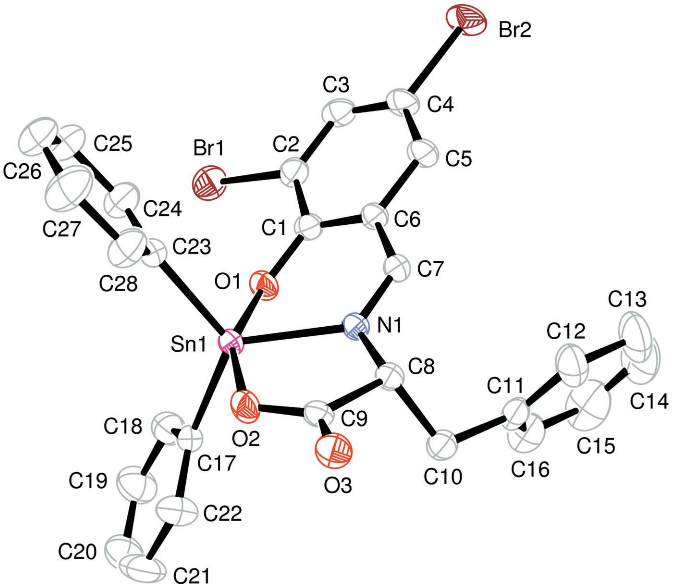


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms omitted for clarity.

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