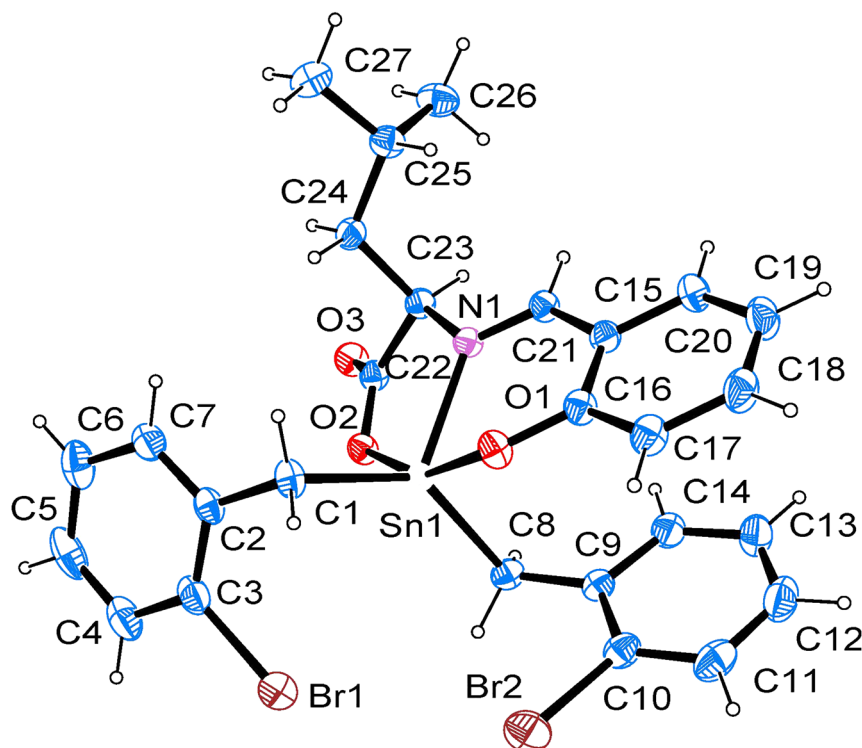


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The crystal structure of bis(2-bromobenzyl)(2-((2-oxybenzylidene)amino)-4-methylpentanoato- $\kappa^3 N, O, O'$)tin(IV), $C_{27}H_{27}Br_2NO_3Sn$



<https://doi.org/10.1515/ncrs-2025-0248>

Received May 27, 2025; accepted July 21, 2025;

published online July 29, 2025

$\beta = 114.2200(10)^\circ$, $\gamma = 108.7940(10)^\circ$, $V = 1329.84(13) \text{ \AA}^3$, $Z = 2$,
 $R_{\text{gt}}(F) = 0.0551$, $wR_{\text{ref}}(F^2) = 0.1538$, $T = 296(2) \text{ K}$.

CCDC no.: 2453228

Abstract

$C_{27}H_{27}Br_2NO_3Sn$, triclinic, $P\bar{1}$ (no. 2), $a = 11.0315(6) \text{ \AA}$,
 $b = 11.5723(7) \text{ \AA}$, $c = 12.3041(7) \text{ \AA}$, $\alpha = 92.1160(10)^\circ$,

The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	$0.19 \times 0.17 \times 0.15 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	3.99 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max} , completeness:	25.1° , 100 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	14050, 4718, 0.019
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4,239
$N(\text{param})_{\text{refined}}$:	307
Programs:	Bruker, ¹ Olex2, ^{2,3} WinGX ⁴

including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of material

All chemicals were purchased from commercial sources and used as received without further purification. An oven-dried flask was charged with salicylidene-leucine (2 mmol), di(2-bromobenzyl)tin dichloride (2 mmol) and CH_3CH_2OH (25 mL). Then, the mixture was refluxed with agitating for 12 h. Finally, the title crystal was precipitated by controlling solvent volatilization.

2 Experimental details

All H-atoms bonded to C atoms were placed geometrically and refined using a riding model with common isotropic displacement factors $U_{iso}(H) = 1.2$ or $1.5 U_{eq}$ (parent C-atom).

3 Comment

Organotin is a kind of widely used main group metal compound, which have more applications than the organic derivatives of any other metal.^{5,6} Due to their biological properties, particularly their possible antitumor activity, organotin(IV) complexes with *O,N,O'*-tridentate Schiff base ligands have garnered attention.^{7–9} Therefore, we conducted research on this kind of organotin compounds.

Single-crystal structure analysis revealed that the title compound crystallized in the centrosymmetric space group $P\bar{1}$. In this complex, the coordination geometry of the tin atom is a twisted triangular bipyramidal shape, with two bromobenzyl and imine N_1 atoms occupying the equatorial positions, and one monodentate carboxylic O_1 atom and phenolic O_2 atom occupying the axial positions.^{10–12} The $Sn1-O2$ bond length is significantly longer than $Sn1-O1$, and the $O1-Sn1-O2$ angle is $157.39(16)^\circ$. The monodentate coordination mode of the carboxylate group is reflected in the disparate $C22-O2$ and $C22-O3$ bond lengths of $1.281(7)$ Å and $1.222(6)$ Å, respectively.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

Research funding: This work was supported by the Research Special Project of Hengyang Normal University (No. KYZX21008, No. KYZX21009), Hunan Provincial Natural Science Foundation of China (No. 2024JJ5057), Scientific Research Projects of Education Department of Hunan Province (No. 23B0669).

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