Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: KH1125). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1997). C**53**, 548–549

Tricyclohexyl[(*N*,*N*-diethylthiocarbamoylthio)acetato-*O*]tin(IV)

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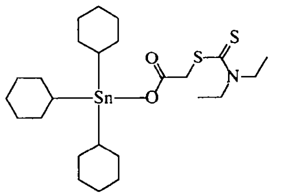
Abstract

The Sn atom in the title compound, [Sn(C_6H_{11})$_3$($C_7H_{12}NO_2S_2$)], is four-coordinate in a distorted tetrahedral arrangement.

Comment

The tricyclohexyltin derivatives of *N*,*N*-dithiocarbamoylacetic acids have been assigned a tetrahedral geometry on the basis of spectroscopic measurements (Ng & Kumar Das, 1991) and this has been confirmed by the present study on the *N*,*N*-diethyldithiocarbamoylacetate derivative, (I). Intermolecular distances exceed 3.5 Å and bond dimensions involving the Sn atom are similar to those found in four-coordinate triorganotin carboxylates (Tiekink, 1991, 1994).



(I)

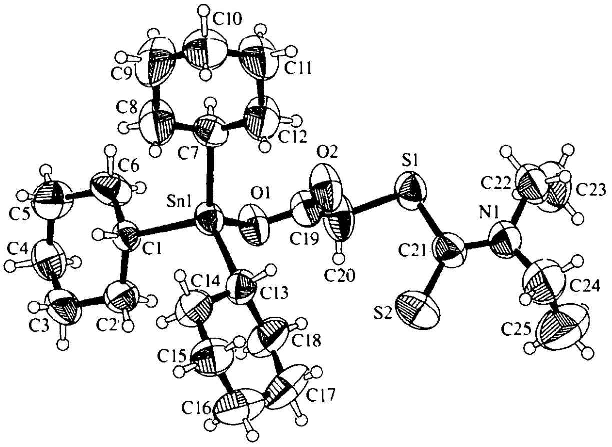


Fig. 1. *ZORTEP* (Zsolnai & Pritzkow, 1996) plot of compound (I). Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

Experimental

The title compound was synthesized from tricyclohexyltin hydroxide and *N*,*N*-diethyldithiocarbamoylacetic acid in ethanol (Ng & Kumar Das, 1991).

Crystal data

[Sn(C_6H_{11})$_3$($C_7H_{12}NO_2S_2$)]
M_r = 574.43
Triclinic
$P\bar{1}$
a = 9.3375 (8) Å
b = 10.0667 (9) Å
c = 17.456 (2) Å
α = 79.866 (9)°
β = 81.874 (9)°
γ = 62.776 (7)°
V = 1432.8 (3) Å^3
Z = 2
D_x = 1.331 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 14.5–15.0°
μ = 1.057 mm^{-1}
T = 300 K
Block
0.51 × 0.43 × 0.36 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer

4451 reflections with $I > 2\sigma(I)$

ω scans
Absorption correction:
ψ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.592$, $T_{\max} = 0.684$
5348 measured reflections
5007 independent reflections

$R_{\rm int} = 0.0117$
$\theta_{\max} = 24.97°$
$h = 0 \rightarrow 11$
$k = -10 \rightarrow 11$
$l = -20 \rightarrow 20$
3 standard reflections
frequency: 60 min
intensity decay: 5.5%

Refinement

Refinement on F^2
$R(F) = 0.0375$
$wR(F^2) = 0.1115$
$S = 1.166$
5004 reflections
280 parameters
H atoms: $U(\rm H) = 1.5U_{\rm eq}(\rm C)$
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 1.028P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.709$ e Å^{-3}
$\Delta\rho_{\min} = -0.281$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Sn1—C1	2.158 (4)	Sn1—C13	2.144 (5)
Sn1—C7	2.149 (4)	Sn1—O1	2.066 (3)
C1—Sn1—C7	110.1 (2)	C7—Sn1—C13	115.5 (2)
C1—Sn1—C13	114.6 (2)	C7—Sn1—O1	113.5 (2)
C1—Sn1—O1	95.2 (1)	C13—Sn1—O1	106.1 (2)

Data collection: *CAD*-4 *VAX/PC* (Enraf–Nonius, 1988). Cell refinement: *CAD*-4 *VAX/PC*. Data reduction: *Xtal*3.0 (Hall & Stewart, 1990). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai & Pritzkow, 1996). Software used to prepare material for publication: *SHELXL*93.

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Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: KH1130). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis[*N*-(4-bromophenyl)salicylaldimine]copper(II)

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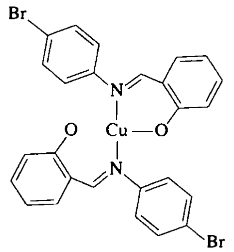
Abstract

The title compound, bis[2-(4-bromophenyliminomethyl)phenolato-*N*,*O*]copper(II), [Cu($C_{13}H_9BrNO$)$_2$], has crystallographic inversion symmetry. The Cu$^{\rm II}$ ion shows a slightly distorted square-planar coordination. The Cu—N and Cu—O distances are 2.019 (4) and 1.879 (4) Å, respectively.

Comment

Metal derivatives of Schiff bases have been extensively studied, and copper(II) and nickel(II) complexes play a major role in both synthetic and structural research. Schiff-base complexes are one of the most important stereochemical models in main group and transition metal coordination chemistry with their easy preparation and structural variation (Garnovskii, Nivorozhkin & Minkin, 1993). Copper(II) and nickel(II) ions react with tridentate anionic Schiff bases, giving dimerized complexes with square-planar configurations (Maggio, Pizzino & Romano, 1974). We report here the results of the reaction of copper(II) with the bidentate ligand *N*-(4-bromophenyl)salicylaldimine, forming the title complex, (I).



(I)

The two bidentate ligands are coordinated as chelates to copper(II). The coordination of the Cu atom is necessarily square planar by symmetry. The Cu—O and Cu—N distances are 1.879 (4) and 2.019 (4) Å, respectively. These distances agree with values in other square-planar coordinated copper(II) complexes (Akhtar