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## Structure of [N-(2-Mercaptophenyl)salicylideneaminato-N,O,S]dimethyltin(IV)

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**Abstract.** [Sn(C<sub>13</sub>H<sub>9</sub>NOS)(CH<sub>3</sub>)<sub>2</sub>],  $M_r = 376.04$ , monoclinic,  $P2_1/n$ ,  $a = 9.623$  (2),  $b = 8.202$  (1),  $c = 18.757$  (3) Å,  $\beta = 96.20$  (1)°,  $V = 1471.79$  (7) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.697$  Mg m<sup>-3</sup>,  $D_m = 1.688$  Mg m<sup>-3</sup> (floatation in chloroform/iodomethane),  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 1.87$  mm<sup>-1</sup>,  $F(000) = 744$ ,  $T = 298$  K,  $R = 0.0456$  for 2505 observed reflections [ $I > 2.5\sigma(I)$ ]. The Sn atom displays a five-coordinate trigonal bipyramidal arrangement in which the tridentate ligand binds to the Sn atom through the O, N and S atoms. The N atom of the ligand and the two methyl groups are located at the equatorial positions. The Sn—O, Sn—N and Sn—S distances are 2.130 (4), 2.176 (4) and 2.554 (1) Å respectively, while the angles O—Sn—N, N—Sn—S and O—Sn—S are 80.6 (1), 77.6 (1) and 158.0 (1)°, respectively.

**Experimental.** The 2-(2-hydroxyphenyl)benzothiazoline was prepared by a previously reported method (Charles & Freiser, 1953). The complex was obtained from a mixture of dimethyltin(IV) dichloride and the ligand in the presence of sodium methoxide. Preliminary data obtained from Weissenberg and Buerger

precession photographs yielded approximate cell dimensions and showed monoclinic symmetry, space group  $P2_1/n$ . Data collection on a crystal  $0.3 \times 0.2 \times 0.2$  mm was performed on a Syntex  $P2_1$  diffractometer in  $2\theta/\theta$  mode ( $0 < h < 12$ ,  $0 < k < 10$ ,  $-20 < l < 20$ ) out to  $2\theta(\text{max.})$  of 52.2°. Variable scan speed of 5.0–29.3° min<sup>-1</sup> was used. Lattice parameters refined using 30 reflections in the range  $35 < 2\theta < 45^\circ$ . Standard reflection  $31\bar{3}$  checked every 50 reflections: no significant deviation. The data were corrected for Lorentz and polarization effects. 3370 reflections were collected, 2970 unique ( $R_{\text{int}} = 0.0243$ ), of which 2505 observed reflections with  $I > 2.5\sigma(I)$  were used for refinement of the structure. Structure solved by direct methods, *SHELXS86* (Sheldrick, 1986), and refined using *SHELX76* (Sheldrick, 1976). Scattering factors for C, H, N, O, S and Sn inlaid in *SHELX76*.

Structure determination and refinement performed on an IBM 4361/4381 computer. Refinement by full-matrix least squares based on  $F$  with idealized riding H atoms (C—H 0.96 Å); anisotropic refinement of non-H atoms, isotropic refinement for H atoms (187 scale, positional and thermal parameters of all the atoms refined in the final cycle). In order to correct the observed structure factors for absorption effects, the program *ABSORB* (Ugozzoli, 1987) was

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Table 1. Atomic coordinates ( $\times 10^4$ ,  $\times 10^5$  for Sn atom) and equivalent isotropic thermal parameters for non-H atoms with *e.s.d.*'s in parentheses

$$B_{eq} = 8\pi^2(U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	$B_{eq}$
Sn	29055 (3)	22146 (4)	1874 (2)	2.9 (2)
S1	1136 (2)	2452 (2)	1104 (1)	4.0 (6)
C1	1411 (5)	4546 (6)	1279 (3)	3.0 (2)
C2	1965 (4)	5537 (6)	780 (2)	2.8 (2)
C3	2162 (6)	7187 (7)	917 (3)	3.7 (3)
C4	1794 (6)	7894 (8)	1542 (3)	4.2 (3)
C5	1254 (7)	6875 (9)	2049 (3)	4.5 (3)
C6	1080 (6)	5237 (9)	1916 (3)	4.4 (3)
N1	2405 (4)	4802 (5)	151 (2)	2.7 (2)
C7	2300 (5)	5639 (7)	-450 (3)	3.3 (2)
C8	2881 (5)	5176 (6)	-1091 (2)	3.1 (2)
C9	3898 (5)	3940 (7)	-1114 (3)	3.2 (2)
C10	4527 (5)	3742 (8)	-1751 (3)	3.9 (2)
C11	4150 (6)	4712 (9)	-2336 (3)	4.4 (3)
C12	3134 (6)	5928 (10)	-2322 (3)	4.5 (3)
C13	2516 (6)	6174 (8)	-1705 (3)	3.9 (2)
O1	4289 (4)	2999 (4)	-557 (2)	3.5 (2)
C14	1672 (6)	811 (8)	-596 (3)	4.2 (3)
C15	4621 (6)	1298 (9)	860 (3)	4.7 (3)

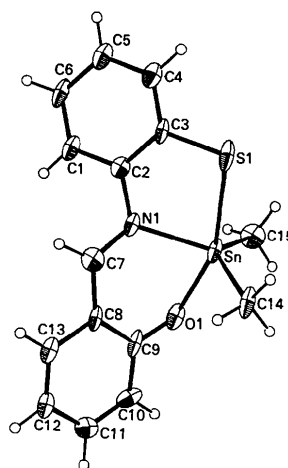


Fig. 1. A perspective view of the molecule.

The atomic parameters for non-H atoms are given in Table 1.\* Table 2 contains bond distances and angles, while the atom-labeling scheme is shown in Fig. 1.

Table 2. Bond distances (Å) and angles (°) with *e.s.d.*'s in parentheses

Sn—S1	2.554 (1)	C5—C4	1.407 (9)
N1—Sn	2.176 (4)	C6—C5	1.373 (10)
O1—Sn	2.130 (4)	C7—N1	1.315 (6)
C14—Sn	2.125 (6)	C8—C7	1.431 (7)
C15—Sn	2.106 (5)	C9—C8	1.413 (7)
C1—S1	1.764 (5)	C13—C8	1.426 (7)
C2—C1	1.389 (6)	C10—C9	1.407 (7)
C6—C1	1.390 (7)	O1—C9	1.321 (6)
C3—C2	1.387 (8)	C11—C10	1.372 (8)
N1—C2	1.428 (6)	C12—C11	1.398 (10)
C4—C3	1.388 (8)	C13—C12	1.371 (7)

N1—Sn—S1	77.6 (1)	C5—C4—C3	118.0 (6)
O1—Sn—S1	158.0 (1)	C6—C5—C4	120.4 (5)
O1—Sn—N1	80.6 (1)	C5—C6—C1	121.3 (6)
C14—Sn—S1	98.2 (2)	C2—N1—Sn	118.0 (3)
C14—Sn—N1	113.7 (2)	C7—N1—Sn	122.2 (3)
C14—Sn—O1	93.0 (2)	C7—N1—C2	119.0 (4)
C15—Sn—S1	99.2 (2)	C8—C7—N1	125.5 (5)
C15—Sn—N1	121.6 (2)	C9—C8—C7	123.5 (4)
C15—Sn—O1	89.7 (2)	C13—C8—C7	116.2 (5)
C15—Sn—C14	124.3 (3)	C13—C8—C9	119.9 (4)
C1—S1—Sn	95.9 (2)	C10—C9—C8	118.2 (5)
C2—C1—S1	120.3 (4)	O1—C9—C8	122.3 (4)
C6—C1—S1	121.0 (4)	O1—C9—C10	119.6 (4)
C6—C1—C2	118.8 (5)	C11—C10—C9	120.8 (5)
C3—C2—C1	120.0 (5)	C12—C11—C10	121.6 (5)
N1—C2—C1	118.7 (4)	C13—C12—C11	119.3 (6)
N1—C2—C3	121.2 (5)	C12—C13—C8	120.3 (5)
C4—C3—C2	121.5 (6)	C9—O1—Sn	123.4 (3)

used (correction factors min.—max.: 0.7973–0.9856). The final agreement factors were  $R = 0.0456$ ,  $wR = 0.0527$ . Weight for every observed structure factor calculated according to  $w = 1.0000/[\sigma^2(F) + 0.007551F^2]$  for which  $S = 1.48$ ,  $(\Delta/\sigma)_{max} = 0.002$ ,  $\Delta\rho_{max} = 1.834$  (near Sn atom) and  $\Delta\rho_{min} = -0.706 \text{ e } \text{Å}^{-3}$ . Geometrical calculations performed with XANADU (Roberts & Sheldrick, 1975) and illustrations drawn with ORTEP (Johnson, 1965).

**Related literature.** Cefalu, Bosco, Bonati, Maggio & Barbieri (1970) reported the synthesis and characterization of the complexes derived from diorganotin(IV) dichloride and 2-(2-hydroxyphenyl)benzothiazoline in a basic medium. The crystal structure of the diphenyltin(IV) complex has been reported (Preut, Haupt, Huber, Cefalu & Barbieri, 1974).

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\* Lists of anisotropic thermal parameters, H-atom parameters, distances and angles involving H atoms, and the observed and calculated structure amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54823 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0115]

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