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[6-(Furan-2-ylideneamino)-1,3-benzothiazole-2-thiolato-κS^2]triphenyltin(IV) ethanol hemisolvate

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The title compound, $[Sn(C_6H_5)_3(C_{12}H_7N_2OS_2)]\cdot 0.5C_2H_6O$, shows a distorted tetrahedral coordination of the Sn atom. The crystal packing is determined by van der Waals interactions.

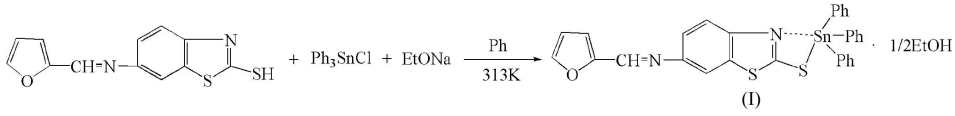
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.012 Å
Disorder in solvent or counterion
R factor = 0.052
wR factor = 0.157
Data-to-parameter ratio = 14.9

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

Comment

Schiff bases still play an important role as ligands in metal coordination chemistry almost a century after their discovery (Sacconi, 1966). Organotin(IV) complexes with Schiff bases have received increasing attention due to their antitumor activities and potential applications in biotechnology (Yang *et al.*, 1999). Triazole derivatives also display a broad range of biological activities, showing potential applications as antitumor, antibacterial, antifungal and antiviral agents (Awad *et al.*, 1991). The crystal structures of a few Schiff bases with the mercaptothiazole unit have been reported in the literature (Yu *et al.*, 2006). We report here the synthesis and structure of the title complex, (I) (Fig. 1).



(I)

The distorted tetrahedral coordination of the Sn atom (Table 1) is characterized by bond angles ranging from 95.30 (18) to 113.45 (17)°. In addition to four coordinated ligands, there is a weak intramolecular interaction Sn1···N1 [2.992 (5) Å].

Experimental

All reagents and solvents were used as purchased without further purification. The reaction was carried out under a nitrogen atmosphere. (*N*-Furanylidene)mercaptobenzothiazole (0.260 g, 1 mmol) was added to a solution in benzene (30 ml) of sodium ethoxide (0.068 g, 1 mmol) in a Schlenk flask; the mixture was stirred for 10 min. Triphenyltin(IV) chloride (0.385 g, 1 mmol) was then added and stirring continued for 12 h at 313 K. After cooling to room temperature, the solution was filtered. The solvent was removed from the filtrate under vacuum, and the solid residue was recrystallized from diethyl ether; yellow crystals suitable for X-ray structure analysis were obtained (yield 85%; m.p. 373–375 K). Analysis calculated for $C_{62}H_{50}N_4O_3S_4Sn_2$: C 58.88, H 3.98, N 4.43%; found: C 58.56, H 3.77, N 4.68%. The elemental analyses were performed with a Perkin–Elmer MODEL 2400 Series II and revealed half a molecule of ethanol per formula unit.

Crystal data

$[Sn(C_6H_5)_3(C_{12}H_7N_2OS_2)]\cdot 0.5C_2H_6O$	$\gamma = 75.145\ (4)^\circ$
$M_r = 632.34$	$V = 1508.8\ (6)\ Å^3$
Triclinic, $P\overline{1}$	$Z = 2$
$a = 9.685\ (2)$ Å	$D_x = 1.392\ Mg\ m^{-3}$
$b = 13.204\ (3)$ Å	Mo $K\alpha$ radiation
$c = 13.323\ (3)$ Å	$\mu = 1.01\ mm^{-1}$
$\alpha = 68.117\ (4)^\circ$	$T = 298\ (2)$ K
$\beta = 76.261\ (4)^\circ$	Block, yellow
	$0.21 \times 0.16 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	8021 measured reflections
φ and ω scans	5267 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3313 reflections with $I > 2\sigma(I)$
$T_{min} = 0.816$, $T_{max} = 0.897$	$R_{int} = 0.030$
	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0829P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.157$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.78$ e Å^{-3}
5267 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
353 parameters	

Table 1
Selected geometric parameters (Å, °).

Sn1—C13	2.129 (7)	Sn1—C19	2.135 (6)
Sn1—C25	2.133 (7)	Sn1—S2	2.460 (2)
C13—Sn1—C25	112.7 (2)	C13—Sn1—S2	112.1 (2)
C13—Sn1—C19	112.6 (2)	C25—Sn1—S2	113.45 (17)
C25—Sn1—C19	109.5 (3)	C19—Sn1—S2	95.30 (18)

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 and O—H = 0.82 Å; $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C,O). According to elemental analysis, the site occupancy factors of the atoms of the ethanol molecule were set at 0.5.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

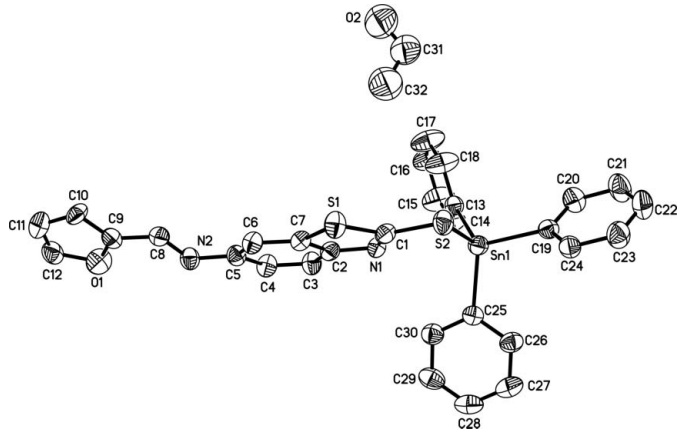


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.

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