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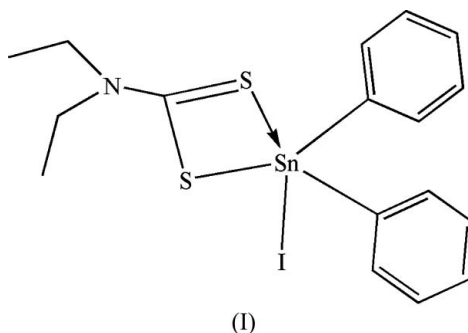
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Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.031
 wR factor = 0.069
Data-to-parameter ratio = 19.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*(N,N*-Diethyldithiocarbamato- κ^2 *S,S')*iododiphenyltin(IV)The Sn atom in the title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_5\text{H}_{10}\text{NS}_2)\text{I}]$, is five-coordinate in a distorted SnIC_2S_2 trigonal-bipyramidal environment.Received 30 August 2006
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Comment

The structures of some chloro- and bromodiorganotin *N,N*-dialkyldithiocarbamates, $R_2\text{Sn}(\text{S}_2\text{CNR}'_2)\text{X}$ ($\text{X} = \text{Cl}, \text{Br}$), have shown that the tin atom exists in a distorted SnXC_2S_2 ($\text{X} = \text{Cl}, \text{Br}$) trigonal-bipyramidal environment (Tiekink, 1992; Tiekink *et al.*, 1999; Yin *et al.*, 2001; Tian *et al.*, 2006). In the iodine-containing title compound, (I), the Sn atom is also five-coordinate and has a distorted trigonal-bipyramidal geometry (Fig. 1 and Table 1). The equatorial plane is defined by atoms C1 and C7 of the phenyl groups and the more tightly held atom S1 of the asymmetrically chelating dithiocarbamate ligand, and the axial positions are occupied by the less tightly held atom S2 and I1, the I1–Sn1–S2 angle being $155.48(3)^\circ$. The Sn atom lies $0.1601(3)\text{ \AA}$ out of the SC_2 trigonal plane in the direction of the I atom. The dihedral angle between the two benzene ring mean planes (C1–C6 and C7–C12) is $89.7(3)^\circ$.



The dithiocarbamate ligand in (I) is anisobidentically chelated to the Sn atom with a difference of $0.2194(10)\text{ \AA}$ between Sn1–S2 and Sn1–S1; the average Sn–S bond distance is $2.5601(10)\text{ \AA}$, which is similar to those found in $\text{Ph}_2\text{Sn}(\text{S}_2\text{CNET}_2)\text{Cl}$ (Dakternieks *et al.*, 1992), $\text{Ph}_2\text{Sn}(\text{S}_2\text{CN-Cy}_2)\text{Cl}$ (Basu Baul & Tiekink, 1993), $\text{Ph}_2\text{Sn}(\text{S}_2\text{CNETCy})\text{Cl}$ (Hall & Tiekink, 1995), $(\text{C}_6\text{H}_5\text{CH}_2)_2\text{Sn}(\text{S}_2\text{CNMe}_2)\text{Cl}$ (Yin *et al.*, 2001) and $\text{Ph}_2\text{Sn}(\text{S}_2\text{CNMe}_2)\text{Br}$ (Tian *et al.*, 2006).

Experimental

A solution of $\text{NaS}_2\text{CN}(\text{C}_2\text{H}_5)_2 \cdot 3\text{H}_2\text{O}$ (0.45 g, 2 mmol) dissolved in methanol (40 ml) was added dropwise to a solution of diphenyltin(IV) diiodide (1.05 g, 2 mmol) in the same solvent (40 ml). The reaction mixture was stirred for about an hour under reflux. The

solvent was removed by using a rotary evaporator. The solid obtained was washed with hot hexane, and then extracted into dichloromethane and filtered. The colorless solid product obtained by removal of dichloromethane was recrystallized from chloroform-ethanol (1:2 v/v) and crystals of (I) were obtained from dichloromethane-hexane (1:1 v/v) by slow evaporation at 298 K (yield 69.7%; m.p. 378–379 K). Analysis found: C 37.25, H 3.67, N 2.56%; calculated for $C_{17}H_{20}INS_2Sn$: C 37.19, H 3.52, N 2.47%.

Crystal data

$[Sn(C_6H_5)_2(C_5H_{10}NS_2)I]$	$V = 996.3 (2) \text{ \AA}^3$
$M_r = 548.05$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.827 \text{ Mg m}^{-3}$
$a = 9.3949 (12) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.9245 (13) \text{ \AA}$	$\mu = 3.04 \text{ mm}^{-1}$
$c = 11.5388 (15) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\alpha = 109.266 (2)^\circ$	Prism, colorless
$\beta = 99.058 (2)^\circ$	$0.19 \times 0.07 \times 0.07 \text{ mm}$
$\gamma = 93.168 (2)^\circ$	

Data collection

Bruker APEX CCD diffractometer	7834 measured reflections
ω scans	3867 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	3245 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.596$, $T_{\max} = 0.816$	$R_{\text{int}} = 0.022$
	$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$
$wR(F^2) = 0.069$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\max} < 0.001$
3867 reflections	$\Delta\rho_{\max} = 0.63 \text{ e \AA}^{-3}$
199 parameters	$\Delta\rho_{\min} = -0.51 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Sn1—C1	2.127 (4)	Sn1—I1	2.8590 (5)
Sn1—C7	2.143 (4)	C13—S1	1.739 (4)
Sn1—S1	2.4504 (10)	C13—S2	1.706 (4)
Sn1—S2	2.6698 (10)		
C1—Sn1—C7	116.91 (14)	S1—Sn1—S2	69.73 (3)
C1—Sn1—S1	120.17 (11)	C1—Sn1—I1	98.52 (10)
C7—Sn1—S1	121.39 (10)	C7—Sn1—I1	98.16 (11)
C1—Sn1—S2	96.04 (11)	S1—Sn1—I1	85.89 (3)
C7—Sn1—S2	92.65 (11)	S2—Sn1—I1	155.48 (3)

H atoms were placed at calculated positions ($C-H = 0.93-0.97 \text{ \AA}$) and refined as riding [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$].

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve

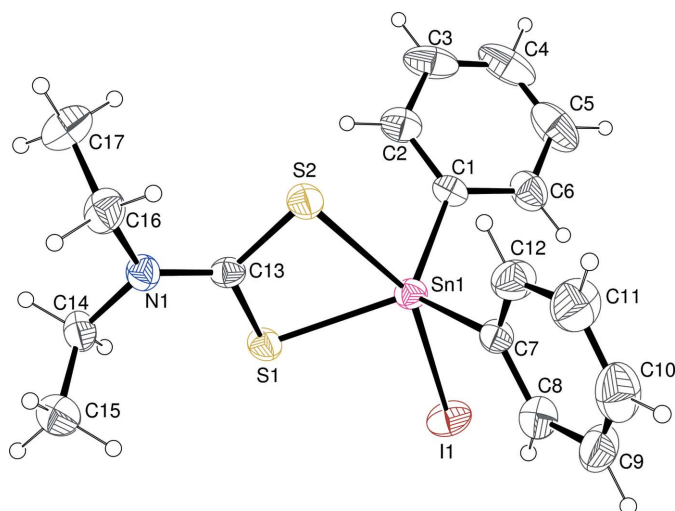


Figure 1

The structure of (I), with displacement ellipsoids drawn at the 30% probability level.

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*.

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