Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(4-Benzylpiperazine-1-carbodithioato)-triphenyltin(IV)

Feng Li, Han-Dong Yin* and Da-Qi Wang

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: handongyin@lctu.edu.cn

Received 17 October 2005
Accepted 27 October 2005
Online 5 November 2005

Key indicators

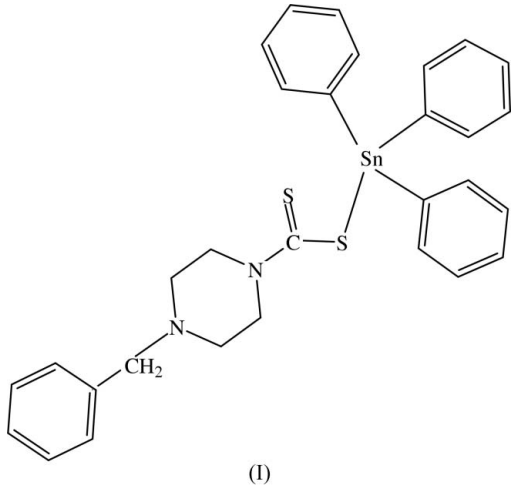
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.010 Å
R factor = 0.043
wR factor = 0.110
Data-to-parameter ratio = 15.3

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

In the title complex, $[Sn(C_6H_6)_3(C_{12}H_{15}N_2S_2)]$, the Sn atom is in a distorted tetrahedral configuration.

Comment

The molecular structure and packing of the title compound, (I), are shown in Figs. 1 and 2, respectively. The Sn atom is surrounded by one S atom of the dithiocarbamate ligand and three C atoms of the phenyl groups in a tetrahedral configuration.



(I)

Experimental

The sodium salt of *N*-benzylpiperazinyldithiocarbamate (0.0906 g, 3.3 mmol) was added to a dichloromethane solution (30 ml) of triphenyltin chloride (1.593 g, 3.0 mmol) and the mixture stirred for 14 h. The sodium chloride which precipitated was removed and the solution concentrated. Diethyl ether (5 ml) and hexane (5 ml) were added to this solution to precipitate the product. The product was recrystallized from a dichloromethane–hexane mixture (1:1 *v*/*v*) to give colourless crystals of (I) (1.45 g, yield 76%, m.p. 446 K). Analysis calculated for $C_{30}H_{30}N_2S_2Sn$: C 59.91, H 5.03, N 4.66, S 10.66%; found: C 60.01, H 4.92, N 4.72, S 10.63%.

Crystal data

$[Sn(C_6H_6)_3(C_{12}H_{15}N_2S_2)]$
M_r = 601.37
Monoclinic, $P2_1/c$
a = 19.063 (4) Å
b = 9.6915 (19) Å
c = 14.968 (3) Å
β = 96.114 (3)°
V = 2749.4 (9) Å^3
Z = 4
D_x = 1.453 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2933 reflections
θ = 2.4–21.3°
μ = 1.10 mm^{-1}
T = 298 (2) K
Block, colourless
0.29 × 0.23 × 0.18 mm

Data collection

Siemens SMART CCD area-detector diffractometer	4831 independent reflections
φ and ω scans	3113 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.050$
$T_{min} = 0.741$, $T_{max} = 0.826$	$\theta_{max} = 25.0^\circ$
14089 measured reflections	$h = -22 \rightarrow 22$
	$k = -11 \rightarrow 8$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 2.1544P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.110$	$\Delta\rho_{max} = 0.73$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.38$ e Å^{-3}
4831 reflections	
316 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C25	2.132 (6)	N1—C2	1.454 (6)
Sn1—C19	2.154 (5)	N2—C4	1.458 (7)
Sn1—C13	2.178 (5)	N2—C3	1.468 (6)
Sn1—S1	2.4858 (15)	N2—C6	1.476 (7)
Sn1—S2	2.9222 (15)	S1—C1	1.738 (5)
N1—C1	1.332 (6)	S2—C1	1.690 (6)
N1—C5	1.453 (7)		
C25—Sn1—C19	115.1 (2)	C25—Sn1—S2	91.05 (15)
C25—Sn1—C13	106.9 (2)	C19—Sn1—S2	85.67 (14)
C19—Sn1—C13	102.42 (19)	C13—Sn1—S2	154.31 (15)
C25—Sn1—S1	106.26 (14)	S1—Sn1—S2	65.33 (5)
C19—Sn1—S1	129.54 (14)	C1—S1—Sn1	94.72 (19)
C13—Sn1—S1	91.56 (14)	C1—S2—Sn1	81.35 (17)

All H atoms were placed in geometrically calculated positions and treated as riding on their parent atoms, with aromatic C—H distances of 0.93 Å and methylene C—H distances of 0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

The authors acknowledge the financial support of the Shandong Province Science Foundation and the State Key Laboratory of Crystal Materials, Shandong University.

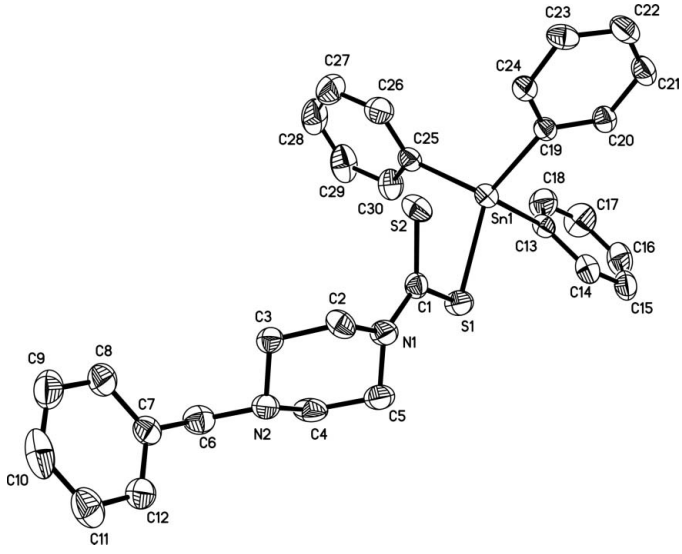


Figure 1
The structure of (I), with 30% probability displacement ellipsoids. H atoms have been omitted.

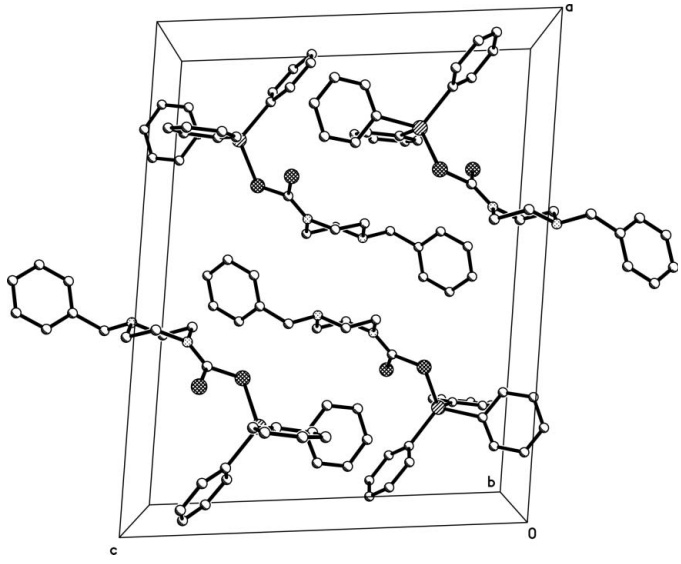


Figure 2
The crystal packing of (I). H atoms have been omitted.

References

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen,Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.