

**(*N*-Butyl-*N*-phenyldithiocarbamato- κ S)-
triphenyltin(IV)**Nurul Farahana Kamaludin,^a Ibrahim Baba,^{b‡} Normah
Awang,^a Mohamed Ibrahim Mohamed Tahir^c and
Edward R. T. Tiekink^{d*}^aEnvironmental Health Programme, Faculty of Allied Health Sciences, Universiti
Kebangsaan Malaysia, Jalan Raja Muda Aziz, 50300 Kuala Lumpur, Malaysia,^bSchool of Chemical Sciences and Food Technology, Faculty of Science and
Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia, ^cDepartment
of Chemistry, Universiti Putra Malaysia, 43400 Serdang, Malaysia, and ^dDepartment
of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: edward.tiekink@gmail.com

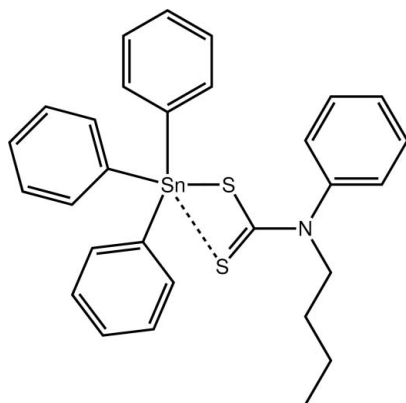
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
R factor = 0.024; wR factor = 0.060; data-to-parameter ratio = 20.4.

The title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{11}\text{H}_{14}\text{NS}_2)]$, features a tetrahedrally coordinated Sn atom, as the dithiocarbamate ligand coordinates in a monodentate fashion. Due to the proximity of the non-coordinating thione S atom, distortions from ideal tetrahedral geometry about the metal atom are evident with the widest C—Sn—S angle being $117.26(5)^\circ$. In the crystal, molecules are linked by C—H \cdots S interactions, which generate helical supramolecular chains along the *b* axis.

Related literature

For a review on the applications and structural chemistry of tin dithiocarbamates, see: Tiekink (2008). For a recently reported related structure, see: Awang *et al.* (2010).

[‡] Additional correspondence author, e-mail: aibi@ukm.my.**Experimental***Crystal data* $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{11}\text{H}_{14}\text{NS}_2)]$
 $M_r = 574.34$ Monoclinic, $P2_1/n$ $a = 10.0488(1)$ Å $b = 18.0008(2)$ Å $c = 15.2054(2)$ Å $\beta = 102.442(1)^\circ$ $V = 2685.85(5)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 1.12$ mm⁻¹ $T = 150$ K $0.24 \times 0.22 \times 0.10$ mm*Data collection*

Oxford Diffraction Xcaliber Eos

Gemini diffractometer

Absorption correction: multi-scan

(CrysAlis PRO; Oxford

Diffraction, 2010)

 $T_{\min} = 0.781$, $T_{\max} = 0.894$

34109 measured reflections

6099 independent reflections

5277 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.044$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.024$ $wR(F^2) = 0.060$ $S = 1.02$

6099 reflections

299 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³**Table 1**

Selected geometric parameters (Å, °).

Sn—S1	2.4772 (5)	Sn—C24	2.1521 (18)
Sn—S2	3.1048 (5)	S1—C1	1.758 (2)
Sn—C12	2.1286 (18)	S2—C1	1.675 (2)
Sn—C18	2.1380 (19)		
C12—Sn—C18	113.76 (7)	C12—Sn—S1	117.26 (5)
C12—Sn—C24	107.51 (7)	C18—Sn—S1	115.54 (5)
C18—Sn—C24	107.45 (7)	C24—Sn—S1	92.18 (5)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C28—H28 \cdots S2 ⁱ	0.95	2.83	3.612 (2)	140

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5836).

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supplementary materials

Acta Cryst. (2011). E67, m555-m556 [doi:10.1107/S1600536811012426]

(*N*-Butyl-*N*-phenyldithiocarbamato- κ S)triphenyltin(IV)

N. F. Kamaludin, I. Baba, N. Awang, M. I. Mohamed Tahir and E. R. T. Tiekink

Comment

Their potential as anti-cancer agents, anti-microbials and insecticides, and as convenient synthetic precursors for tin sulfide nanoparticles, attract continued attention to organotin dithiocarbamates (Tiekink, 2008). As part of on-going of structural studies of triphenyltin(IV) dithiocarbamates (Awang *et al.*, 2010), the analysis of the title compound, (I), was undertaken.

The molecular structure, Fig. 1, features Sn coordinated by the dithiocarbamate ligand and three *ipso*-C atoms of three benzene rings. The dithiocarbamate ligand coordinates essentially in a monodentate fashion, an assignment supported by the large disparity in the C—S bond distances, Table 1. The coordination geometry is based on a tetrahedron with the range of tetrahedral angles being 92.18 (5) to 117.26 (5)°. The wider angles are ascribed to the influence of the proximate S2 atom. The crystal packing of (I) features helical supramolecular chains along the *b* axis that is sustained by C—H...S interactions, Fig. 2 and Table 2.

Experimental

The title compound was prepared using an *in situ* method by the addition of carbon disulfide (0.01 mol) to an ethanolic solution of *N*-butylphenylamine (0.01 mol). The mixture was stirred for 1 h at 277 K. The solution was then added drop-wise to a solution of triphenyltin(IV) chloride (0.01 mol) in ethanol (20 ml). The mixture was stirred for 1 h. The white precipitate that formed was filtered, washed with cold ethanol and dried in a desiccator. Crystallization was carried out by using an ethanol:chloroform (1:1 *v/v*) mixture to yield colourless prisms of (I). Yield: 34%. *M.pt.* 374–375 K. Elemental analysis. Found (calculated) for C₂₉H₂₉NS₂Sn: C, 60.54 (60.64); H 5.08 (5.09); N 2.34 (2.44); S 11.31 (11.17); Sn 20.19 (20.66)%. UV (CHCl₃) λ_{\max} 252 nm ($L(\pi) \rightarrow L(\pi^*)$). IR (KBr): $\nu(\text{C—H})$ 2960 m; $\nu(\text{C}\cdots\text{N})$ 1477 m; $\nu(\text{N—C})$ 1139 s; $\nu(\text{C}\cdots\text{S})$ 997 s; $\nu(\text{Cd—S})$ 356 s cm⁻¹.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to 1.2 to 1.5 $U_{\text{equiv}}(\text{C})$.

Figures

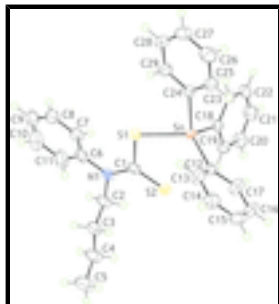


Fig. 1. The molecular structure of (I) showing the displacement ellipsoids at the 50% probability level.

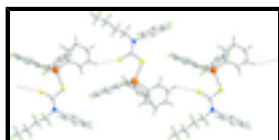


Fig. 2. A view of the helical supramolecular chain in (I) mediated by C—H...S interactions (orange dashed lines) along the *b* axis in (I).

(*N*-Butyl-*N*-phenyldithiocarbamato- κ S)triphenyltin(IV)

Crystal data

[Sn(C₆H₅)₃(C₁₁H₁₄NS₂)]

M_r = 574.34

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2yn

a = 10.0488 (1) Å

b = 18.0008 (2) Å

c = 15.2054 (2) Å

β = 102.442 (1)°

V = 2685.85 (5) Å³

Z = 4

F(000) = 1168

D_x = 1.420 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 18395 reflections

θ = 2–29°

μ = 1.12 mm⁻¹

T = 150 K

Prism, colourless

0.24 × 0.22 × 0.10 mm

Data collection

Oxford Diffraction Xcaliber Eos Gemini diffractometer

Radiation source: fine-focus sealed tube graphite

Detector resolution: 16.1952 pixels mm⁻¹

ω scans

Absorption correction: multi-scan (*Crys.Alis PRO*; Oxford Diffraction, 2010)

T_{min} = 0.781, *T_{max}* = 0.894

34109 measured reflections

6099 independent reflections

5277 reflections with *I* > 2 σ (*I*)

R_{int} = 0.044

θ_{\max} = 27.5°, θ_{\min} = 2.2°

h = -13→13

k = -23→23

l = -19→19

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.024$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.060$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.6995P]$
6099 reflections	where $P = (F_o^2 + 2F_c^2)/3$
299 parameters	$(\Delta/\sigma)_{\max} = 0.003$
0 restraints	$\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn	0.636843 (12)	0.514323 (7)	0.706567 (8)	0.02366 (5)
S1	0.74819 (5)	0.56428 (3)	0.85614 (3)	0.03110 (11)
S2	0.60687 (5)	0.42144 (3)	0.87326 (3)	0.03087 (11)
N1	0.72072 (18)	0.50776 (9)	1.01112 (11)	0.0316 (4)
C1	0.6917 (2)	0.49591 (10)	0.92221 (13)	0.0280 (4)
C2	0.6806 (2)	0.45399 (12)	1.07424 (13)	0.0366 (5)
H2A	0.5941	0.4299	1.0445	0.044*
H2B	0.6642	0.4811	1.1276	0.044*
C3	0.7875 (2)	0.39454 (12)	1.10512 (14)	0.0392 (5)
H3A	0.8713	0.4180	1.1404	0.047*
H3B	0.8106	0.3705	1.0518	0.047*
C4	0.7378 (3)	0.33576 (13)	1.16269 (15)	0.0471 (6)
H4A	0.6524	0.3135	1.1280	0.057*
H4B	0.7172	0.3597	1.2168	0.057*
C5	0.8423 (3)	0.27455 (16)	1.19190 (19)	0.0671 (8)
H5A	0.8668	0.2525	1.1386	0.101*
H5B	0.8035	0.2362	1.2247	0.101*
H5C	0.9239	0.2955	1.2312	0.101*

supplementary materials

C6	0.7940 (2)	0.57343 (12)	1.05062 (13)	0.0338 (5)
C7	0.7210 (2)	0.63472 (12)	1.06800 (14)	0.0365 (5)
H7	0.6242	0.6337	1.0544	0.044*
C8	0.7902 (3)	0.69796 (13)	1.10562 (15)	0.0442 (5)
H8	0.7407	0.7403	1.1178	0.053*
C9	0.9303 (3)	0.69916 (15)	1.12510 (15)	0.0518 (6)
H9	0.9775	0.7427	1.1498	0.062*
C10	1.0025 (3)	0.63747 (16)	1.10886 (17)	0.0578 (7)
H10	1.0993	0.6384	1.1228	0.069*
C11	0.9344 (2)	0.57402 (15)	1.07221 (15)	0.0485 (6)
H11	0.9842	0.5312	1.0620	0.058*
C12	0.71232 (19)	0.41209 (10)	0.66655 (12)	0.0258 (4)
C13	0.8499 (2)	0.40110 (12)	0.67362 (15)	0.0377 (5)
H13	0.9118	0.4400	0.6962	0.045*
C14	0.8999 (2)	0.33402 (12)	0.64823 (16)	0.0442 (5)
H14	0.9952	0.3274	0.6540	0.053*
C15	0.8124 (3)	0.27783 (12)	0.61507 (15)	0.0421 (5)
H15	0.8465	0.2319	0.5986	0.050*
C16	0.6745 (3)	0.28803 (12)	0.60564 (17)	0.0498 (6)
H16	0.6132	0.2494	0.5811	0.060*
C17	0.6240 (2)	0.35448 (12)	0.63171 (15)	0.0404 (5)
H17	0.5285	0.3607	0.6257	0.048*
C18	0.41962 (19)	0.52313 (10)	0.67250 (13)	0.0263 (4)
C19	0.3332 (2)	0.47347 (11)	0.70304 (14)	0.0329 (4)
H19	0.3709	0.4336	0.7413	0.039*
C20	0.1932 (2)	0.48155 (13)	0.67828 (17)	0.0439 (6)
H20	0.1357	0.4477	0.7004	0.053*
C21	0.1365 (2)	0.53874 (15)	0.62151 (17)	0.0489 (6)
H21	0.0403	0.5446	0.6052	0.059*
C22	0.2205 (2)	0.58712 (13)	0.58878 (15)	0.0426 (5)
H22	0.1819	0.6256	0.5485	0.051*
C23	0.3614 (2)	0.57999 (11)	0.61427 (13)	0.0328 (4)
H23	0.4184	0.6140	0.5919	0.039*
C24	0.71761 (18)	0.60219 (10)	0.63749 (12)	0.0260 (4)
C25	0.7478 (2)	0.59142 (12)	0.55345 (14)	0.0388 (5)
H25	0.7282	0.5450	0.5238	0.047*
C26	0.8063 (3)	0.64789 (14)	0.51222 (16)	0.0510 (6)
H26	0.8271	0.6395	0.4550	0.061*
C27	0.8344 (2)	0.71606 (13)	0.55379 (16)	0.0472 (6)
H27	0.8737	0.7546	0.5252	0.057*
C28	0.8049 (3)	0.72759 (12)	0.63682 (16)	0.0455 (6)
H28	0.8242	0.7743	0.6659	0.055*
C29	0.7472 (2)	0.67142 (11)	0.67806 (14)	0.0383 (5)
H29	0.7272	0.6802	0.7355	0.046*

Atomic displacement parameters (\AA^2)

U^{11}

U^{22}

U^{33}

U^{12}

U^{13}

U^{23}

Sn	0.02646 (8)	0.02098 (8)	0.02380 (8)	-0.00103 (5)	0.00594 (5)	-0.00096 (5)
S1	0.0410 (3)	0.0271 (2)	0.0234 (2)	-0.0021 (2)	0.0029 (2)	0.00049 (19)
S2	0.0389 (3)	0.0250 (2)	0.0299 (2)	0.0037 (2)	0.0100 (2)	0.00173 (19)
N1	0.0396 (10)	0.0330 (9)	0.0223 (8)	0.0080 (7)	0.0072 (7)	0.0010 (7)
C1	0.0301 (10)	0.0281 (10)	0.0259 (10)	0.0106 (8)	0.0061 (8)	0.0028 (8)
C2	0.0456 (12)	0.0418 (12)	0.0253 (10)	0.0110 (10)	0.0138 (9)	0.0053 (9)
C3	0.0446 (13)	0.0421 (12)	0.0316 (11)	0.0116 (10)	0.0101 (10)	0.0074 (9)
C4	0.0654 (16)	0.0486 (14)	0.0314 (11)	0.0150 (12)	0.0196 (11)	0.0083 (10)
C5	0.087 (2)	0.0596 (17)	0.0554 (17)	0.0233 (16)	0.0181 (15)	0.0239 (14)
C6	0.0410 (12)	0.0404 (12)	0.0194 (9)	0.0069 (9)	0.0051 (8)	0.0001 (8)
C7	0.0408 (12)	0.0376 (12)	0.0317 (11)	0.0069 (9)	0.0091 (9)	0.0032 (9)
C8	0.0604 (15)	0.0376 (12)	0.0352 (12)	0.0068 (11)	0.0111 (11)	-0.0012 (10)
C9	0.0596 (16)	0.0566 (15)	0.0342 (12)	-0.0082 (13)	-0.0009 (11)	-0.0076 (11)
C10	0.0419 (14)	0.078 (2)	0.0483 (15)	0.0000 (13)	-0.0023 (12)	-0.0180 (14)
C11	0.0415 (13)	0.0615 (16)	0.0389 (13)	0.0146 (11)	0.0005 (10)	-0.0115 (11)
C12	0.0340 (10)	0.0218 (9)	0.0230 (9)	-0.0014 (8)	0.0090 (8)	0.0004 (7)
C13	0.0342 (11)	0.0316 (11)	0.0468 (13)	-0.0021 (9)	0.0076 (10)	-0.0081 (9)
C14	0.0435 (13)	0.0396 (12)	0.0501 (14)	0.0115 (10)	0.0111 (11)	-0.0039 (11)
C15	0.0688 (16)	0.0272 (11)	0.0359 (12)	0.0091 (11)	0.0238 (11)	0.0014 (9)
C16	0.0684 (17)	0.0299 (12)	0.0554 (15)	-0.0169 (11)	0.0226 (13)	-0.0156 (11)
C17	0.0415 (12)	0.0348 (12)	0.0482 (13)	-0.0096 (9)	0.0171 (10)	-0.0120 (10)
C18	0.0270 (9)	0.0280 (10)	0.0234 (9)	0.0008 (7)	0.0046 (8)	-0.0057 (7)
C19	0.0310 (10)	0.0334 (11)	0.0344 (11)	-0.0019 (8)	0.0073 (9)	0.0015 (9)
C20	0.0322 (11)	0.0515 (14)	0.0491 (14)	-0.0063 (10)	0.0111 (10)	-0.0004 (11)
C21	0.0295 (11)	0.0597 (15)	0.0526 (15)	0.0049 (11)	-0.0017 (11)	-0.0041 (12)
C22	0.0413 (12)	0.0402 (12)	0.0402 (12)	0.0093 (10)	-0.0045 (10)	-0.0001 (10)
C23	0.0393 (11)	0.0291 (10)	0.0276 (10)	-0.0006 (9)	0.0023 (9)	-0.0013 (8)
C24	0.0265 (9)	0.0249 (9)	0.0253 (9)	-0.0006 (7)	0.0025 (8)	0.0026 (7)
C25	0.0540 (14)	0.0325 (11)	0.0312 (11)	-0.0070 (10)	0.0122 (10)	-0.0023 (9)
C26	0.0723 (17)	0.0504 (15)	0.0358 (12)	-0.0063 (13)	0.0237 (12)	0.0062 (11)
C27	0.0547 (14)	0.0398 (13)	0.0481 (14)	-0.0105 (11)	0.0131 (12)	0.0156 (11)
C28	0.0639 (15)	0.0261 (11)	0.0432 (13)	-0.0108 (10)	0.0046 (12)	0.0037 (9)
C29	0.0588 (14)	0.0265 (10)	0.0308 (11)	-0.0036 (10)	0.0122 (10)	-0.0013 (8)

Geometric parameters (Å, °)

Sn—S1	2.4772 (5)	C12—C13	1.377 (3)
Sn—S2	3.1048 (5)	C12—C17	1.393 (3)
Sn—C12	2.1286 (18)	C13—C14	1.394 (3)
Sn—C18	2.1380 (19)	C13—H13	0.9500
Sn—C24	2.1521 (18)	C14—C15	1.364 (3)
S1—C1	1.758 (2)	C14—H14	0.9500
S2—C1	1.675 (2)	C15—C16	1.374 (3)
N1—C1	1.337 (2)	C15—H15	0.9500
N1—C6	1.453 (3)	C16—C17	1.390 (3)
N1—C2	1.479 (3)	C16—H16	0.9500
C2—C3	1.517 (3)	C17—H17	0.9500
C2—H2A	0.9900	C18—C19	1.394 (3)
C2—H2B	0.9900	C18—C23	1.396 (3)

supplementary materials

C3—C4	1.524 (3)	C19—C20	1.384 (3)
C3—H3A	0.9900	C19—H19	0.9500
C3—H3B	0.9900	C20—C21	1.385 (3)
C4—C5	1.521 (3)	C20—H20	0.9500
C4—H4A	0.9900	C21—C22	1.378 (3)
C4—H4B	0.9900	C21—H21	0.9500
C5—H5A	0.9800	C22—C23	1.391 (3)
C5—H5B	0.9800	C22—H22	0.9500
C5—H5C	0.9800	C23—H23	0.9500
C6—C11	1.378 (3)	C24—C25	1.389 (3)
C6—C7	1.382 (3)	C24—C29	1.394 (3)
C7—C8	1.391 (3)	C25—C26	1.390 (3)
C7—H7	0.9500	C25—H25	0.9500
C8—C9	1.375 (3)	C26—C27	1.381 (3)
C8—H8	0.9500	C26—H26	0.9500
C9—C10	1.377 (4)	C27—C28	1.373 (3)
C9—H9	0.9500	C27—H27	0.9500
C10—C11	1.385 (4)	C28—C29	1.382 (3)
C10—H10	0.9500	C28—H28	0.9500
C11—H11	0.9500	C29—H29	0.9500
C12—Sn—C18	113.76 (7)	C13—C12—C17	118.00 (18)
C12—Sn—C24	107.51 (7)	C13—C12—Sn	121.01 (14)
C18—Sn—C24	107.45 (7)	C17—C12—Sn	120.99 (15)
C12—Sn—S1	117.26 (5)	C12—C13—C14	121.2 (2)
C18—Sn—S1	115.54 (5)	C12—C13—H13	119.4
C24—Sn—S1	92.18 (5)	C14—C13—H13	119.4
C1—S1—Sn	97.64 (7)	C15—C14—C13	120.1 (2)
C1—N1—C6	121.91 (17)	C15—C14—H14	119.9
C1—N1—C2	121.41 (18)	C13—C14—H14	119.9
C6—N1—C2	116.68 (16)	C16—C15—C14	119.7 (2)
N1—C1—S2	123.79 (16)	C16—C15—H15	120.2
N1—C1—S1	116.04 (15)	C14—C15—H15	120.2
S2—C1—S1	120.16 (12)	C15—C16—C17	120.5 (2)
N1—C2—C3	112.88 (17)	C15—C16—H16	119.8
N1—C2—H2A	109.0	C17—C16—H16	119.8
C3—C2—H2A	109.0	C16—C17—C12	120.5 (2)
N1—C2—H2B	109.0	C16—C17—H17	119.8
C3—C2—H2B	109.0	C12—C17—H17	119.8
H2A—C2—H2B	107.8	C19—C18—C23	118.40 (18)
C2—C3—C4	111.70 (18)	C19—C18—Sn	123.25 (14)
C2—C3—H3A	109.3	C23—C18—Sn	118.31 (14)
C4—C3—H3A	109.3	C20—C19—C18	120.8 (2)
C2—C3—H3B	109.3	C20—C19—H19	119.6
C4—C3—H3B	109.3	C18—C19—H19	119.6
H3A—C3—H3B	107.9	C19—C20—C21	120.4 (2)
C3—C4—C5	112.3 (2)	C19—C20—H20	119.8
C3—C4—H4A	109.1	C21—C20—H20	119.8
C5—C4—H4A	109.1	C22—C21—C20	119.5 (2)
C3—C4—H4B	109.1	C22—C21—H21	120.2

C5—C4—H4B	109.1	C20—C21—H21	120.2
H4A—C4—H4B	107.9	C21—C22—C23	120.5 (2)
C4—C5—H5A	109.5	C21—C22—H22	119.8
C4—C5—H5B	109.5	C23—C22—H22	119.8
H5A—C5—H5B	109.5	C22—C23—C18	120.4 (2)
C4—C5—H5C	109.5	C22—C23—H23	119.8
H5A—C5—H5C	109.5	C18—C23—H23	119.8
H5B—C5—H5C	109.5	C25—C24—C29	117.65 (18)
C11—C6—C7	120.5 (2)	C25—C24—Sn	121.76 (14)
C11—C6—N1	120.44 (19)	C29—C24—Sn	120.53 (14)
C7—C6—N1	119.07 (19)	C24—C25—C26	120.7 (2)
C6—C7—C8	119.5 (2)	C24—C25—H25	119.7
C6—C7—H7	120.2	C26—C25—H25	119.7
C8—C7—H7	120.2	C27—C26—C25	120.5 (2)
C9—C8—C7	120.0 (2)	C27—C26—H26	119.7
C9—C8—H8	120.0	C25—C26—H26	119.7
C7—C8—H8	120.0	C28—C27—C26	119.5 (2)
C8—C9—C10	120.2 (2)	C28—C27—H27	120.3
C8—C9—H9	119.9	C26—C27—H27	120.3
C10—C9—H9	119.9	C29—C28—C27	120.1 (2)
C9—C10—C11	120.2 (2)	C29—C28—H28	120.0
C9—C10—H10	119.9	C27—C28—H28	120.0
C11—C10—H10	119.9	C28—C29—C24	121.6 (2)
C6—C11—C10	119.6 (2)	C28—C29—H29	119.2
C6—C11—H11	120.2	C24—C29—H29	119.2
C10—C11—H11	120.2		
C12—Sn—S1—C1	-68.43 (8)	C13—C14—C15—C16	0.9 (4)
C18—Sn—S1—C1	70.03 (8)	C14—C15—C16—C17	-1.6 (4)
C24—Sn—S1—C1	-179.43 (8)	C15—C16—C17—C12	1.0 (4)
C6—N1—C1—S2	-179.67 (14)	C13—C12—C17—C16	0.4 (3)
C2—N1—C1—S2	0.9 (3)	Sn—C12—C17—C16	179.86 (17)
C6—N1—C1—S1	0.3 (2)	C12—Sn—C18—C19	58.98 (18)
C2—N1—C1—S1	-179.14 (14)	C24—Sn—C18—C19	177.86 (16)
Sn—S1—C1—N1	-173.43 (14)	S1—Sn—C18—C19	-80.93 (16)
Sn—S1—C1—S2	6.51 (12)	C12—Sn—C18—C23	-118.75 (14)
C1—N1—C2—C3	88.8 (2)	C24—Sn—C18—C23	0.13 (16)
C6—N1—C2—C3	-90.7 (2)	S1—Sn—C18—C23	101.34 (14)
N1—C2—C3—C4	-174.46 (18)	C23—C18—C19—C20	-1.8 (3)
C2—C3—C4—C5	178.3 (2)	Sn—C18—C19—C20	-179.52 (16)
C1—N1—C6—C11	-87.1 (2)	C18—C19—C20—C21	0.9 (4)
C2—N1—C6—C11	92.3 (2)	C19—C20—C21—C22	0.8 (4)
C1—N1—C6—C7	94.2 (2)	C20—C21—C22—C23	-1.7 (4)
C2—N1—C6—C7	-86.3 (2)	C21—C22—C23—C18	0.8 (3)
C11—C6—C7—C8	1.5 (3)	C19—C18—C23—C22	0.9 (3)
N1—C6—C7—C8	-179.84 (18)	Sn—C18—C23—C22	178.78 (15)
C6—C7—C8—C9	0.1 (3)	C12—Sn—C24—C25	29.77 (18)
C7—C8—C9—C10	-1.1 (4)	C18—Sn—C24—C25	-93.05 (17)
C8—C9—C10—C11	0.5 (4)	S1—Sn—C24—C25	149.29 (16)
C7—C6—C11—C10	-2.1 (3)	C12—Sn—C24—C29	-147.32 (16)

supplementary materials

N1—C6—C11—C10	179.2 (2)	C18—Sn—C24—C29	89.86 (17)
C9—C10—C11—C6	1.1 (4)	S1—Sn—C24—C29	-27.81 (16)
C18—Sn—C12—C13	172.10 (15)	C29—C24—C25—C26	0.5 (3)
C24—Sn—C12—C13	53.25 (18)	Sn—C24—C25—C26	-176.71 (18)
S1—Sn—C12—C13	-48.72 (17)	C24—C25—C26—C27	-0.6 (4)
C18—Sn—C12—C17	-7.36 (19)	C25—C26—C27—C28	0.5 (4)
C24—Sn—C12—C17	-126.21 (16)	C26—C27—C28—C29	-0.2 (4)
S1—Sn—C12—C17	131.82 (15)	C27—C28—C29—C24	0.1 (4)
C17—C12—C13—C14	-1.1 (3)	C25—C24—C29—C28	-0.2 (3)
Sn—C12—C13—C14	179.44 (17)	Sn—C24—C29—C28	177.00 (17)
C12—C13—C14—C15	0.5 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C28—H28 \cdots S2 ⁱ	0.95	2.83	3.612 (2)	140

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$.

Fig. 1

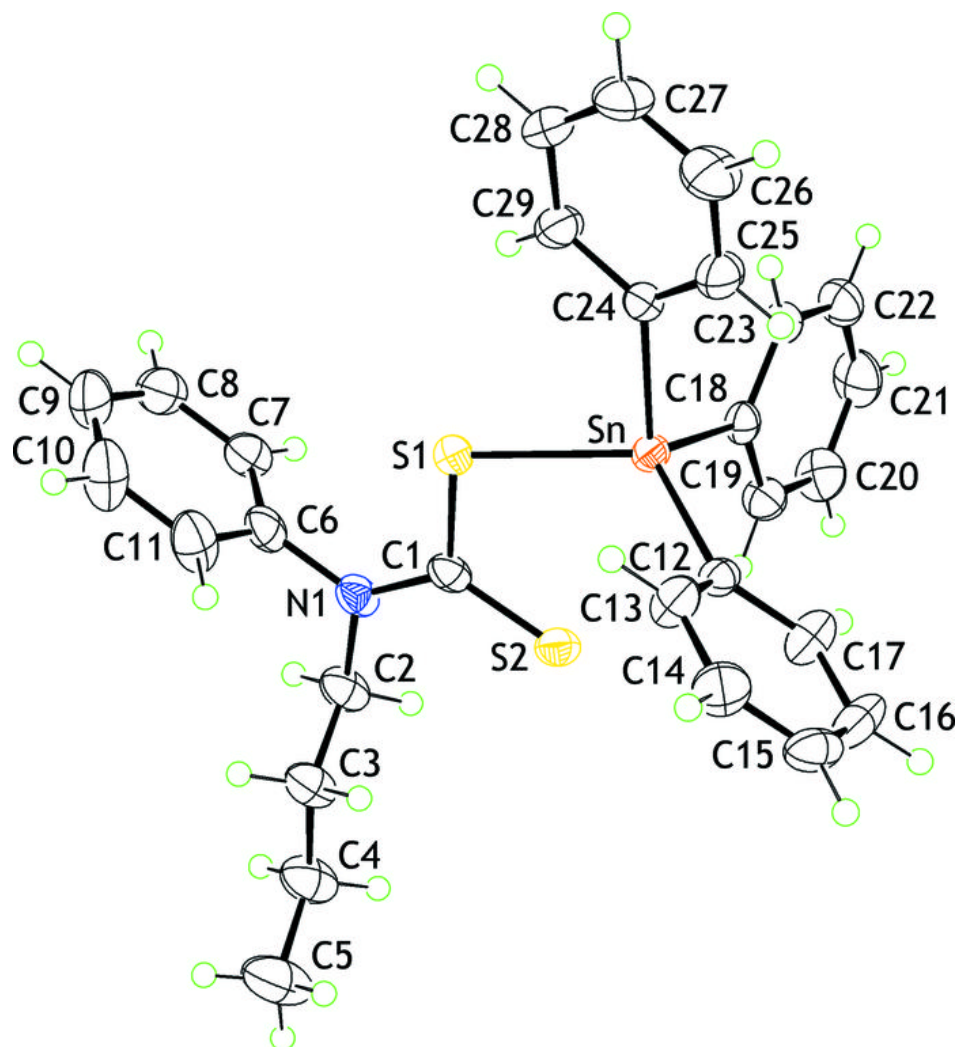


Fig. 2

