

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(Dimethyl sulfoxide- κ O)diphenyl(3-thioxo-3H-1,2-dithiole-4,5-dithiolato- κ^2 S⁴,S⁵)tin(IV)

Nadia M. Comerlato,^a Edward R. T. Tiekink,^{b*} James L. Wardell^{c‡} and Solange M. S. V. Wardell^d

^aDepartamento de Química Inorgânica, Instituto de Química, Universidade Federal do Rio de Janeiro, CP 68563, 21941-909 Rio de Janeiro, RJ, Brazil, ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, ^cCentro de Desenvolvimento Tecnológico em Saúde (CDTS), Fundação Oswaldo Cruz (FIOCRUZ), Casa Amarela, Campus de Manguinhos, Av. Brasil 4365, 21040-900, Rio de Janeiro, RJ, Brazil, and ^dCHEMSOL, 1 Harcourt Road, Aberdeen AB15 5NY, Scotland

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

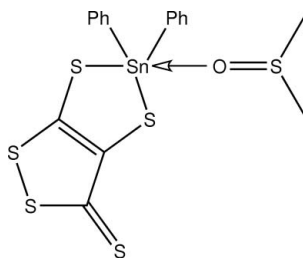
Received 7 November 2009; accepted 11 November 2009

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 20.9.

The Sn atom in the title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_3\text{S}_5)(\text{C}_2\text{H}_6\text{OS})]$, exists within a distorted trigonal-bipyramidal geometry defined by two S atoms of the 1,2-dithiole-3-thione-4,5-dithiolate dianion, two *ipso*-C atoms from the phenyl groups, and the O atom of the dimethyl sulfoxide molecule. In this description, one of the S atoms and the O occupy axial positions. In the crystal, centrosymmetrically related molecules associate *via* pairs of $\text{C}-\text{H}\cdots\text{S}$ contacts, forming dimeric aggregates.

Related literature

For background to the synthesis of dmt compounds, see: Steimecke *et al.* (1982). For related crystal structures, see: Aupers *et al.* (1998); Khan *et al.* (1998); Chohan *et al.* (1999); Bordinhão *et al.* (2006, 2008); Comerlato *et al.* (2008). For additional analysis of geometry, see: Addison *et al.* (1984).



‡ Additional correspondence author: j.wardell@abdn.ac.uk.

Experimental

Crystal data

$[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_3\text{S}_5)(\text{C}_2\text{H}_6\text{OS})]$
 $M_r = 547.35$
 Monoclinic, $P2_1/n$
 $a = 11.1420$ (5) Å
 $b = 15.7237$ (6) Å
 $c = 11.9646$ (6) Å
 $\beta = 96.892$ (2)°
 $V = 2080.97$ (16) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.83$ mm⁻¹
 $T = 120$ K
 $0.24 \times 0.16 \times 0.10$ mm

Data collection

Bruker–Nonius 95mm CCD camera
 on κ -goniostat diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2007)
 $T_{\min} = 0.536$, $T_{\max} = 0.746$
 22729 measured reflections
 4770 independent reflections
 3906 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.088$
 $S = 1.06$
 4770 reflections
 228 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.85$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.26$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sn–C4	2.130 (3)	Sn–S1	2.4357 (9)
Sn–C10	2.133 (3)	Sn–S2	2.5582 (9)
Sn–O1	2.311 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{S2}^i$	0.95	2.71	3.599 (4)	157

Symmetry code: (i) $-x + 2, -y, -z$.

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2009).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England, and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES (Brazil).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5220).

References

- Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
 Aupers, J. H., Chohan, Z. H., Cox, P. J., Doidge-Harrison, S. M. S. V., Howie, R. A., Khan, A., Spencer, G. M. & Wardell, J. L. (1998). *Polyhedron*, **17**, 4475–4486.

- Bordinhão, J., Comerlato, N. M., de Castro Cortás, L., Ferreira, G. B., Howie, R. A. & Wardell, J. L. (2008). *J. Organomet. Chem.* **693**, 763–768.
- Bordinhão, J., Comerlato, N. M., Ferreira, G. B., Howie, R. A., da Silva, C. X. A. & Wardell, J. L. (2006). *J. Organomet. Chem.* **691**, 1598–1605.
- Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Chohan, Z. H., Howie, R. A. & Wardell, J. L. (1999). *J. Organomet. Chem.* **577**, 140–149.
- Comerlato, N. M., Ferreira, G. B., Howie, R. A., Silva, C. X. A. & Wardell, J. L. (2008). *J. Organomet. Chem.* **693**, 2424–2430.
- Hoof, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Khan, A., Low, J. N., Wardell, J. L. & Ferguson, G. (1998). *Acta Cryst.* **C54**, 1399–1401.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (2007). *SADABS*. Version 2007/2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Steimecke, G., Sieler, H.-J., Kirmse, R., Dietzch, W. & Hoyer, E. (1982). *Phosphorus Sulfur*, **12**, 237–247.
- Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E65, m1592–m1593 [doi:10.1107/S1600536809047904]

(Dimethyl sulfoxide- κ O)diphenyl(3-thioxo-3H-1,2-dithiole-4,5-dithiolato- κ^2 S⁴,S⁵)tin(IV)

Nadia M. Comerlato, Edward R. T. Tiekink, James L. Wardell and Solange M. S. V. Wardell

S1. Comment

While several structures of (1,3-dithiole-2-thione-4,5-dithiolato)tin, [Sn-dmit], and (1,3-dithiole-2-one-4,5-dithiolato)tin [Sn-dmio] complexes have been reported (*e.g.*, Comerlato *et al.*, 2008), similar (1,2-dithiole-3-thione-4,5-dithiolato)tin complexes have been essentially neglected, with only one systematic study known (Bordinhão *et al.*, 2006; Bordinhão *et al.*, 2008); see Fig. 1 for chemical structures of dmit, dmio and dmt. The poor solubility of 1,2-dithiole-3-thione-4,5-dithiolato (dmt) complexes has been put forward as a major cause for the limited number of their reported crystal structures. Attempts to obtain good crystals of Ph₂Sn(dmt), prepared from reaction of Na₂(dmt) and Ph₂SnCl₂ in MeOH solution, failed as only amorphous material was obtained. However, crystallization of Ph₂Sn(dmt) from a DMSO/MeOH solution produced crystals of the DMSO solvate, (I), suitable for the X-Ray study reported herein.

As compounds, R₂Sn(dmit) and R₂Sn(dmio), having non-functionalized alkyl or aryl R groups (*e.g.*, R = Me, Et, Bu or Ph), are aggregated in both the solid-state and in non-coordinating solvents as a consequence of intermolecular Sn...S interactions., it is assumed that the R₂Sn(dmt) analogues are similarly aggregated. The formation of adducts such as [Ph₂Sn(dmt)(dmsO)] will generally provide coordinatively saturated tin centres and hence result in appreciably more soluble species having essentially non-interacting cations and anions. Structures of ionic species, [Q][R₂Sn(dmit)X] and [Q][R₂Sn(dmio)X] [Q+ = onium cation, X = halide or pseudohalide], with 5-coordinate tin have also been determined (Chohan *et al.*, 1999; Khan *et al.*, 1998; Aupers *et al.*, 1998).

The Sn atom in (I) is five-coordinate, existing within a C₂OS₂ donor set defined by a chelating dmt ligand, two *ipso*-C atoms and the O atom derived from the DMSO molecule, Fig. 2. The coordination geometry is based on a trigonal bipyramid with the S2–Sn–O1 axial angle being 166.52 (6) °. As expected, the Sn–S1_{equatorial} distance of 2.4357 (9) Å is shorter than the Sn–S2_{axial} distance of 2.5582 (9) Å. The coordination geometry is distorted towards trigonal bipyramidal (TP). This is quantified by the value of $\tau = 0.72$, which compares with the ideal values of 1.0 and 0.0 for TP and square pyramidal, respectively (Addison *et al.*, 1984).

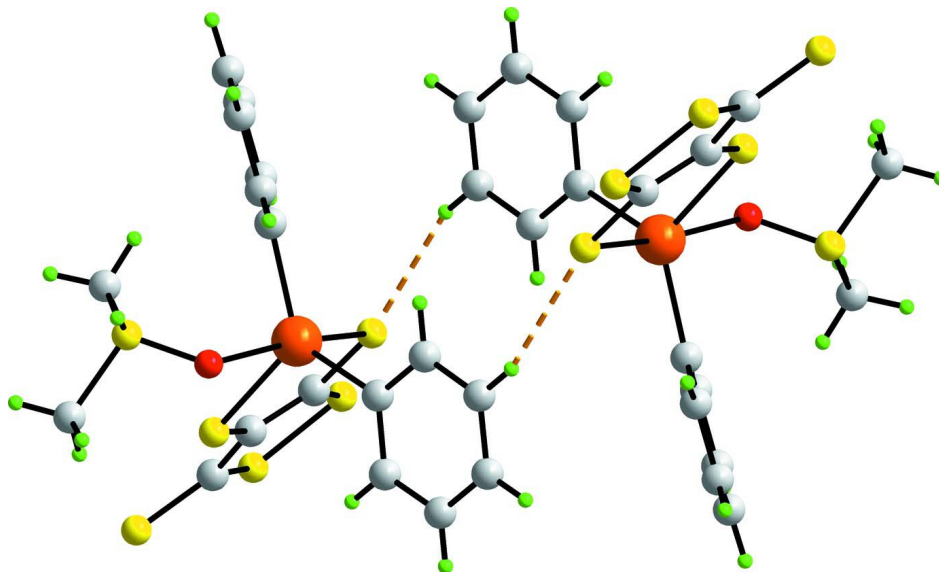
The most prominent intermolecular interaction connecting molecules is of the type C–H...S and these occur between centrosymmetric pairs to form loosely associated dimers, Table 1 and Fig. 3.

S2. Experimental

To a stirred suspension of 4,5-bis(benzoylthio)-1,2-dithiole-3-thione (Steimecke *et al.*, 1982) (410 mg, 1 mmol) in methanol (10 ml), under argon, was added a sodium methoxide solution prepared from sodium (150 mg, 6.75 mmol) and methanol (10 ml). To the resulting purple solution of Na₂dmt was added with stirring a methanolic solution of Ph₂SnCl₂ (345 mg, 1 mmol). The reaction mixture was stirred for 1 h, rotary evaporated and the residue washed well with water. The solid residue (535 mg) was dissolved in a mixture of DMSO and MeOH (*ca* v:v 3:1) and left to slowly recrystallize to give (I); m.pt. 428–431 K (dec.) IR (KBr, cm⁻¹): 1061 (ν C–S), 950, 941 (ν S–O), 910, 827, 720 (ν C=S).

Figure 2

Molecular structure (I) showing displacement ellipsoids at the 50% probability level.

**Figure 3**

Supramolecular dimer in (I) mediated by C–H⋯S contacts (orange dashed lines). Colour code: Sn, orange; S, yellow; O, red; C, grey; and H, green.

(Dimethyl sulfoxide- κ O)diphenyl(3-thioxo-3H-1,2-dithiole-4,5-dithiolato- κ^2 S⁴,S⁵)tin(IV)

Crystal data

[Sn(C₆H₅)₂(C₃S₅)(C₂H₆OS)]

$M_r = 547.35$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 11.1420$ (5) Å

$b = 15.7237$ (6) Å

$c = 11.9646$ (6) Å

$\beta = 96.892$ (2)°

$V = 2080.97$ (16) Å³

$Z = 4$

$F(000) = 1088$

$D_x = 1.747$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 44319 reflections

$\theta = 2.9$ – 27.5°

$\mu = 1.83$ mm⁻¹

$T = 120$ K

Block, yellow

$0.24 \times 0.16 \times 0.10$ mm

Data collection

Bruker–Nonius 95mm CCD camera on κ -goniostat

diffractometer

Radiation source: Bruker–Nonius FR591

rotating anode

Graphite monochromator

Detector resolution: 9.091 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2007)

$T_{\min} = 0.536$, $T_{\max} = 0.746$

22729 measured reflections

4770 independent reflections

3906 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -14 \rightarrow 14$

$k = -20 \rightarrow 19$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.088$
 $S = 1.06$
 4770 reflections
 228 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 1.7706P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.85 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.26 \text{ e } \text{Å}^{-3}$

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 (Å^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn	0.823308 (19)	0.079364 (13)	0.201486 (19)	0.01886 (9)
S1	0.64254 (8)	0.07006 (5)	0.29688 (7)	0.02196 (18)
S2	0.68225 (8)	0.10256 (6)	0.01905 (8)	0.0263 (2)
S3	0.42347 (8)	0.12813 (5)	-0.02069 (8)	0.0266 (2)
S4	0.30214 (8)	0.12492 (6)	0.09713 (8)	0.0302 (2)
S5	0.35612 (8)	0.08574 (6)	0.33685 (9)	0.0301 (2)
S6	0.89763 (8)	0.13614 (5)	0.46902 (8)	0.0264 (2)
O1	0.9096 (2)	0.06287 (13)	0.38570 (19)	0.0218 (5)
C1	0.5279 (3)	0.09377 (19)	0.1865 (3)	0.0210 (7)
C2	0.5481 (3)	0.1063 (2)	0.0763 (3)	0.0226 (7)
C3	0.4068 (3)	0.0995 (2)	0.2126 (3)	0.0249 (7)
C4	0.8953 (3)	-0.0427 (2)	0.1706 (3)	0.0199 (7)
C5	1.0061 (3)	-0.0547 (2)	0.1308 (3)	0.0291 (8)
H5	1.0562	-0.0073	0.1200	0.035*
C6	1.0440 (3)	-0.1366 (2)	0.1067 (3)	0.0349 (9)
H6	1.1200	-0.1448	0.0798	0.042*
C7	0.9712 (3)	-0.2061 (2)	0.1217 (3)	0.0327 (9)
H7	0.9965	-0.2616	0.1037	0.039*
C8	0.8622 (3)	-0.1945 (2)	0.1626 (3)	0.0277 (8)
H8	0.8126	-0.2423	0.1735	0.033*
C9	0.8241 (3)	-0.1133 (2)	0.1883 (3)	0.0216 (7)
H9	0.7495	-0.1059	0.2179	0.026*
C10	0.9274 (3)	0.1927 (2)	0.1953 (3)	0.0212 (7)
C11	1.0477 (3)	0.1947 (2)	0.2438 (3)	0.0260 (7)
H11	1.0842	0.1443	0.2758	0.031*

C12	1.1145 (3)	0.2691 (2)	0.2459 (3)	0.0331 (9)
H12	1.1963	0.2698	0.2792	0.040*
C13	1.0608 (4)	0.3427 (2)	0.1990 (4)	0.0376 (10)
H13	1.1055	0.3943	0.2023	0.045*
C14	0.9438 (4)	0.3415 (2)	0.1480 (3)	0.0350 (9)
H14	0.9085	0.3919	0.1147	0.042*
C15	0.8763 (3)	0.2666 (2)	0.1450 (3)	0.0270 (8)
H15	0.7956	0.2658	0.1087	0.032*
C16	1.0469 (3)	0.1532 (2)	0.5361 (3)	0.0351 (9)
H16A	1.0823	0.0987	0.5628	0.053*
H16B	1.0443	0.1917	0.6002	0.053*
H16C	1.0962	0.1785	0.4824	0.053*
C17	0.8353 (4)	0.0869 (3)	0.5831 (4)	0.0423 (10)
H17A	0.7533	0.0670	0.5574	0.064*
H17B	0.8326	0.1281	0.6441	0.064*
H17C	0.8858	0.0384	0.6105	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.01908 (13)	0.01369 (12)	0.02314 (14)	0.00039 (8)	-0.00013 (9)	0.00187 (8)
S1	0.0222 (4)	0.0193 (4)	0.0241 (5)	0.0009 (3)	0.0015 (3)	0.0028 (3)
S2	0.0210 (4)	0.0330 (5)	0.0243 (5)	0.0008 (3)	0.0000 (4)	0.0059 (4)
S3	0.0213 (4)	0.0276 (4)	0.0293 (5)	0.0011 (3)	-0.0039 (4)	0.0000 (4)
S4	0.0194 (4)	0.0347 (5)	0.0356 (5)	0.0019 (4)	-0.0007 (4)	-0.0036 (4)
S5	0.0259 (5)	0.0298 (5)	0.0360 (6)	-0.0008 (3)	0.0096 (4)	-0.0007 (4)
S6	0.0326 (5)	0.0183 (4)	0.0263 (5)	0.0038 (3)	-0.0041 (4)	-0.0022 (3)
O1	0.0270 (13)	0.0153 (11)	0.0224 (13)	0.0015 (9)	0.0004 (10)	-0.0005 (9)
C1	0.0199 (16)	0.0128 (15)	0.0292 (19)	0.0002 (12)	-0.0021 (14)	-0.0015 (13)
C2	0.0222 (17)	0.0168 (15)	0.0276 (19)	0.0021 (13)	-0.0011 (14)	-0.0005 (13)
C3	0.0210 (17)	0.0190 (16)	0.034 (2)	-0.0001 (13)	-0.0012 (15)	-0.0006 (14)
C4	0.0210 (16)	0.0172 (15)	0.0203 (17)	0.0019 (13)	-0.0024 (13)	0.0010 (13)
C5	0.0271 (19)	0.0246 (17)	0.036 (2)	0.0000 (14)	0.0059 (16)	0.0053 (16)
C6	0.031 (2)	0.041 (2)	0.035 (2)	0.0111 (17)	0.0121 (17)	0.0045 (17)
C7	0.044 (2)	0.0218 (17)	0.032 (2)	0.0098 (16)	0.0041 (17)	-0.0024 (15)
C8	0.039 (2)	0.0174 (16)	0.0254 (19)	-0.0013 (14)	0.0002 (16)	0.0044 (14)
C9	0.0221 (17)	0.0195 (16)	0.0222 (18)	-0.0016 (13)	-0.0013 (14)	0.0008 (13)
C10	0.0257 (17)	0.0170 (15)	0.0216 (18)	-0.0003 (13)	0.0063 (14)	-0.0002 (13)
C11	0.0243 (17)	0.0233 (17)	0.030 (2)	-0.0018 (14)	0.0027 (15)	-0.0018 (14)
C12	0.029 (2)	0.034 (2)	0.038 (2)	-0.0086 (16)	0.0099 (17)	-0.0065 (17)
C13	0.049 (3)	0.0236 (18)	0.045 (2)	-0.0145 (17)	0.026 (2)	-0.0081 (17)
C14	0.050 (2)	0.0178 (17)	0.041 (2)	0.0041 (16)	0.021 (2)	0.0026 (16)
C15	0.0300 (19)	0.0197 (16)	0.032 (2)	0.0039 (14)	0.0051 (15)	0.0014 (14)
C16	0.035 (2)	0.033 (2)	0.034 (2)	-0.0047 (16)	-0.0112 (17)	0.0022 (17)
C17	0.049 (3)	0.049 (3)	0.031 (2)	-0.0049 (19)	0.012 (2)	-0.0018 (18)

Geometric parameters (Å, °)

Sn—C4	2.130 (3)	C7—C8	1.375 (5)
Sn—C10	2.133 (3)	C7—H7	0.9500
Sn—O1	2.311 (2)	C8—C9	1.392 (5)
Sn—S1	2.4357 (9)	C8—H8	0.9500
Sn—S2	2.5582 (9)	C9—H9	0.9500
S1—C1	1.764 (3)	C10—C11	1.396 (5)
S2—C2	1.718 (3)	C10—C15	1.398 (5)
S3—C2	1.734 (3)	C11—C12	1.386 (5)
S3—S4	2.0674 (13)	C11—H11	0.9500
S4—C3	1.744 (4)	C12—C13	1.390 (6)
S5—C3	1.667 (4)	C12—H12	0.9500
S6—O1	1.540 (2)	C13—C14	1.372 (6)
S6—C16	1.778 (4)	C13—H13	0.9500
S6—C17	1.781 (4)	C14—C15	1.395 (5)
C1—C2	1.379 (5)	C14—H14	0.9500
C1—C3	1.423 (5)	C15—H15	0.9500
C4—C5	1.388 (5)	C16—H16A	0.9800
C4—C9	1.395 (5)	C16—H16B	0.9800
C5—C6	1.396 (5)	C16—H16C	0.9800
C5—H5	0.9500	C17—H17A	0.9800
C6—C7	1.384 (5)	C17—H17B	0.9800
C6—H6	0.9500	C17—H17C	0.9800
C4—Sn—C10	121.97 (12)	C6—C7—H7	120.0
C4—Sn—O1	86.68 (10)	C7—C8—C9	120.3 (3)
C10—Sn—O1	87.79 (10)	C7—C8—H8	119.8
C4—Sn—S1	112.16 (9)	C9—C8—H8	119.8
C10—Sn—S1	123.38 (9)	C8—C9—C4	120.2 (3)
O1—Sn—S1	79.58 (6)	C8—C9—H9	119.9
C4—Sn—S2	100.73 (9)	C4—C9—H9	119.9
C10—Sn—S2	97.58 (9)	C11—C10—C15	118.8 (3)
O1—Sn—S2	166.52 (6)	C11—C10—Sn	120.2 (2)
S1—Sn—S2	87.16 (3)	C15—C10—Sn	121.0 (2)
C1—S1—Sn	101.66 (12)	C12—C11—C10	120.9 (3)
C2—S2—Sn	98.03 (12)	C12—C11—H11	119.6
C2—S3—S4	94.35 (12)	C10—C11—H11	119.6
C3—S4—S3	96.65 (12)	C11—C12—C13	119.5 (4)
O1—S6—C16	104.84 (17)	C11—C12—H12	120.3
O1—S6—C17	104.05 (17)	C13—C12—H12	120.3
C16—S6—C17	98.6 (2)	C14—C13—C12	120.5 (3)
S6—O1—Sn	118.36 (12)	C14—C13—H13	119.7
C2—C1—C3	117.9 (3)	C12—C13—H13	119.7
C2—C1—S1	124.0 (3)	C13—C14—C15	120.3 (3)
C3—C1—S1	118.0 (3)	C13—C14—H14	119.9
C1—C2—S2	128.8 (3)	C15—C14—H14	119.9
C1—C2—S3	117.3 (3)	C14—C15—C10	120.0 (3)

S2—C2—S3	113.9 (2)	C14—C15—H15	120.0
C1—C3—S5	128.2 (3)	C10—C15—H15	120.0
C1—C3—S4	113.7 (3)	S6—C16—H16A	109.5
S5—C3—S4	118.1 (2)	S6—C16—H16B	109.5
C5—C4—C9	119.3 (3)	H16A—C16—H16B	109.5
C5—C4—Sn	123.5 (2)	S6—C16—H16C	109.5
C9—C4—Sn	117.2 (2)	H16A—C16—H16C	109.5
C4—C5—C6	120.0 (3)	H16B—C16—H16C	109.5
C4—C5—H5	120.0	S6—C17—H17A	109.5
C6—C5—H5	120.0	S6—C17—H17B	109.5
C7—C6—C5	120.3 (3)	H17A—C17—H17B	109.5
C7—C6—H6	119.9	S6—C17—H17C	109.5
C5—C6—H6	119.9	H17A—C17—H17C	109.5
C8—C7—C6	119.9 (3)	H17B—C17—H17C	109.5
C8—C7—H7	120.0		
C4—Sn—S1—C1	-105.26 (14)	O1—Sn—C4—C5	-94.0 (3)
C10—Sn—S1—C1	92.39 (15)	S1—Sn—C4—C5	-171.4 (3)
O1—Sn—S1—C1	172.71 (12)	S2—Sn—C4—C5	97.3 (3)
S2—Sn—S1—C1	-4.83 (10)	C10—Sn—C4—C9	173.5 (2)
C4—Sn—S2—C2	116.74 (14)	O1—Sn—C4—C9	88.2 (3)
C10—Sn—S2—C2	-118.59 (14)	S1—Sn—C4—C9	10.8 (3)
O1—Sn—S2—C2	-5.7 (3)	S2—Sn—C4—C9	-80.5 (2)
S1—Sn—S2—C2	4.72 (11)	C9—C4—C5—C6	1.4 (5)
C2—S3—S4—C3	-1.58 (16)	Sn—C4—C5—C6	-176.4 (3)
C16—S6—O1—Sn	-130.43 (17)	C4—C5—C6—C7	0.3 (6)
C17—S6—O1—Sn	126.56 (19)	C5—C6—C7—C8	-1.3 (6)
C4—Sn—O1—S6	177.97 (16)	C6—C7—C8—C9	0.5 (6)
C10—Sn—O1—S6	55.76 (16)	C7—C8—C9—C4	1.2 (5)
S1—Sn—O1—S6	-68.78 (13)	C5—C4—C9—C8	-2.2 (5)
S2—Sn—O1—S6	-58.2 (3)	Sn—C4—C9—C8	175.8 (3)
Sn—S1—C1—C2	4.4 (3)	C4—Sn—C10—C11	-42.9 (3)
Sn—S1—C1—C3	-176.2 (2)	O1—Sn—C10—C11	41.8 (3)
C3—C1—C2—S2	-179.4 (3)	S1—Sn—C10—C11	117.8 (2)
S1—C1—C2—S2	0.0 (5)	S2—Sn—C10—C11	-150.6 (3)
C3—C1—C2—S3	0.1 (4)	C4—Sn—C10—C15	138.4 (3)
S1—C1—C2—S3	179.45 (17)	O1—Sn—C10—C15	-136.9 (3)
Sn—S2—C2—C1	-4.1 (3)	S1—Sn—C10—C15	-60.9 (3)
Sn—S2—C2—S3	176.36 (15)	S2—Sn—C10—C15	30.7 (3)
S4—S3—C2—C1	1.1 (3)	C15—C10—C11—C12	2.3 (5)
S4—S3—C2—S2	-179.35 (16)	Sn—C10—C11—C12	-176.4 (3)
C2—C1—C3—S5	178.8 (3)	C10—C11—C12—C13	-0.1 (6)
S1—C1—C3—S5	-0.6 (4)	C11—C12—C13—C14	-1.8 (6)
C2—C1—C3—S4	-1.6 (4)	C12—C13—C14—C15	1.4 (6)
S1—C1—C3—S4	179.03 (17)	C13—C14—C15—C10	0.9 (5)
S3—S4—C3—C1	2.0 (2)	C11—C10—C15—C14	-2.7 (5)
S3—S4—C3—S5	-178.38 (18)	Sn—C10—C15—C14	176.0 (3)
C10—Sn—C4—C5	-8.7 (4)		

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>
C6—H6 \cdots S2 ⁱ	0.95	2.71	3.599 (4)	157

Symmetry code: (i) $-x+2, -y, -z$.