



# [*N*-Benzyl-*N*-(2-phenylethyl)dithiocarbamato- $\kappa^2S,S'$ ]triphenyltin(IV) and [bis(2-methoxyethyl)dithiocarbamato- $\kappa^2S,S'$ ]triphenyltin(IV): crystal structures and Hirshfeld surface analysis

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Received 20 September 2016

Accepted 21 September 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

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**Keywords:** crystal structure; organotin; dithiocarbamate; Hirshfeld surface analysis.

**CCDC references:** 1505733; 1505732

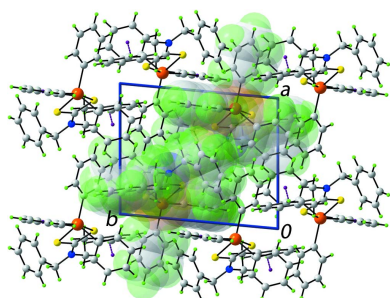
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The crystal and molecular structures of two triphenyltin dithiocarbamates, [Sn(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>(C<sub>16</sub>H<sub>16</sub>NS<sub>2</sub>)], (I), and [Sn(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>(C<sub>7</sub>H<sub>14</sub>NO<sub>2</sub>S<sub>2</sub>)], (II), are described. In (I), the dithiocarbamate ligand coordinates the Sn<sup>IV</sup> atom in an asymmetric manner, leading to a highly distorted trigonal–bipyramidal coordination geometry defined by a C<sub>3</sub>S<sub>2</sub> donor set with the weakly bound S atom approximately *trans* to one of the *ipso*-C atoms. A similar structure is found in (II), but the dithiocarbamate ligand coordinates in an even more asymmetric fashion. The packing in (I) features supramolecular chains along the *c* axis sustained by C–H·· $\pi$  interactions; chains pack with no directional interactions between them. In (II), supramolecular layers are formed, similarly sustained by C–H·· $\pi$  interactions; these stack along the *b* axis. An analysis of the Hirshfeld surfaces for (I) and (II) confirms the presence of the C–H·· $\pi$  interactions but also reveals the overall dominance of H·· $\pi$  contacts in the respective crystals.

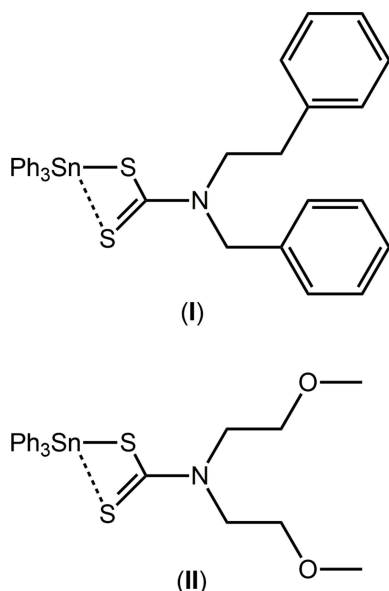
## 1. Chemical context

Among the varied motivations for investigating organotin dithiocarbamate compounds, *i.e.* R<sub>*n*</sub>Sn(S<sub>2</sub>CNRR')<sub>4-*n*</sub> where R, R' = alkyl, aryl, most relate to their biological activities and their usefulness as molecular, single-source precursors for the formation of tin sulfide nanoparticles (Tiekink, 2008). In terms of the latter, while triorganotin dithiocarbamates, *i.e.* with *n* = 3, have been examined in this context (Kana *et al.*, 2001), di- and mono-organotin derivatives often provide more effective precursors (Ramasamy *et al.*, 2013). By contrast, significant interest in the biological effects of triorganotin dithiocarbamates continues. Hence, a wide variety of biological applications of triorganotin dithiocarbamates, *i.e.* directly related to the title compounds, have been investigated. Thus, anti-bacterial (Muthalib *et al.*, 2015), larvicidal (Song *et al.*, 2004), including against mosquito larvae (Basu Baul *et al.*, 2005), insecticidal (Awang *et al.*, 2012; Safari *et al.*, 2013) and anti-leishmanial activities (Ali *et al.*, 2014) have been investigated. However, most activity has been directed towards evaluating their potential as anti-cancer agents (Tiekink, 2008; Khan *et al.*, 2014, 2015). It was in this context and during ongoing structural studies of organotin dithiocarbamates



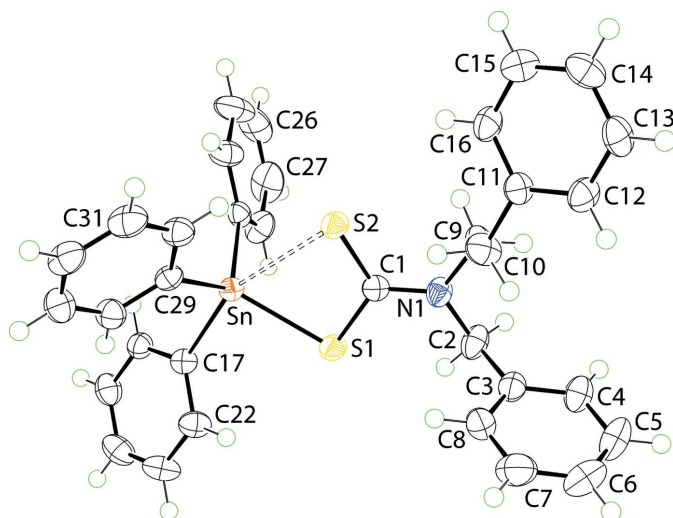
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(Muthalib *et al.*, 2014; Mohamad *et al.*, 2016) that the title compounds were synthesized. Herein, the crystal and molecular structures of  $(\text{C}_6\text{H}_5)_3\text{Sn}[\text{S}_2\text{CN}(\text{Ben})\text{CH}_2\text{CH}_2\text{Ph}]$  (I) and  $(\text{C}_6\text{H}_5)_3\text{Sn}[\text{S}_2\text{CN}(\text{CH}_2\text{CH}_2\text{OMe})_2]$  (II) are reported along with a detailed analysis of the supramolecular association operating in their crystal structures by means of Hirshfeld surface analysis.



### 1.1. Structural commentary

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are collected in Table 1. The tin atom is bound to three phenyl groups and to the dithiocarbamate ligand. The latter coordinates asymmetrically with  $\Delta(\text{Sn}-\text{S})$ , being the difference between the  $\text{Sn}-\text{S}_{\text{long}}$  and  $\text{Sn}-\text{S}_{\text{short}}$  bond lengths, of 0.42 Å. This asymmetry is reflected in the relatively large disparity in the associated C–S bond lengths with the bond involving the tightly bound S1 atom



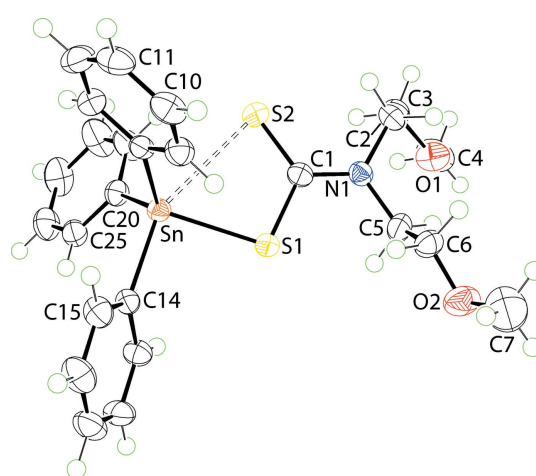
**Figure 1**  
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

**Table 1**  
Geometric data (Å, °) for (I) and (II).

Parameter	(I)	(II)
Sn–S1	2.4886 (4)	2.4612 (4)
Sn–S2	2.9120 (3)	3.0992 (4)
Sn–C17	2.1696 (13)	–
Sn–C23	2.1309 (13)	–
Sn–C29	2.1469 (13)	–
Sn–C8	–	2.1312 (14)
Sn–C14	–	2.1608 (14)
Sn–C20	–	2.1357 (15)
C1–S1	1.7532 (13)	1.7629 (14)
C1–S2	1.6902 (13)	1.6781 (14)
S1–Sn–S2	65.919 (10)	63.534 (11)
S2–Sn–C17	158.55 (4)	–
S2–Sn–C14	–	154.45 (4)

being significantly longer than the bond involving the S2 atom, Table 1. Such a great difference might imply a monodentate mode of coordination for the dithiocarbamate ligand and the adoption of a tetrahedral coordination geometry. However, the range of tetrahedral angles if this were the case is over 30°, *i.e.* from a narrow 92.98 (4)° for S1–Sn–C17 to a wide 124.31 (4)° for S1–Sn–C29. The wide angle is due to the close approach to the tin atom of S2. Further, the Sn–C17 bond length is systematically longer than the other Sn–C bond lengths, an observation ascribed to the C17 atom being approximately *trans* to the incoming S2 atom, Table 1. Thus, the coordination geometry is best described as being based on a  $\text{C}_3\text{S}_2$  donor set. The geometry is not ideal with the value of  $\tau$  of 0.57, *cf.*  $\tau$  values of 0.0 and 1.0 for ideal square-pyramidal and trigonal-bipyramidal geometries, respectively (Addison *et al.*, 1984), suggesting a small distortion towards trigonal-bipyramidal. Distortions from the ideal can be related to the disparate Sn–donor atom bond lengths and the acute chelate angle, Table 1.

The molecular structure of (II) (Fig. 2) bears many similarities with that just described for (I). The value of  $\Delta(\text{Sn}-\text{S})$  of



**Figure 2**  
The molecular structure of (II), showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level. Only the major component of the disordered C5–C6–O2–C7 chain is shown, where atoms C6 and O2 are split over two positions.

Table 2

Hydrogen-bond geometry (Å, °) for (I).

$Cg1$  and  $Cg2$  are the centroids of the C17–C22 and C23–C28 rings, respectively.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C4-H4 \cdots Cg1^i$	0.95	2.63	3.4732 (17)	148
$C13-H13 \cdots Cg2^{ii}$	0.95	2.62	3.5227 (17)	159

Symmetry codes: (i)  $-x + 1, -y + 1, -z$ ; (ii)  $x, y, z + 1$ .

0.64 Å is even greater than that of (I), indicating a more asymmetric mode of coordination of the dithiocarbamate ligand. This difference is also reflected in the associated C–S bond lengths, following the same trend as for (I) but, with  $\Delta(C-S)$  of 0.08 Å *cf.* 0.06 Å for (I). This being stated, the Sn–C14 bond length of 2.1608 (14)°, with the C14 atom being *trans* to the S2 atom, is the longest of all six Sn–C bonds in (I) and (II). The range of tetrahedral angles, *i.e.* 90.94 (4)° for S1–Sn–C14 to 119.54 (5)° for C8–Sn–C20, is slightly narrower at less than 30°. The value of  $\tau$  computes to 0.58, *i.e.* virtually identical to that in (I).

## 2. Supramolecular features

Despite there being five aromatic rings in the molecule of (I), the closest face-to-face contact between rings is > 4.0 Å. The only points of contact between molecules in the molecular packing identified by *PLATON* (Spek, 2009) are those of the type C–H··· $\pi$ . Each of the rings of the dithiocarbamate ligand donates a hydrogen atom to a different tin-bound

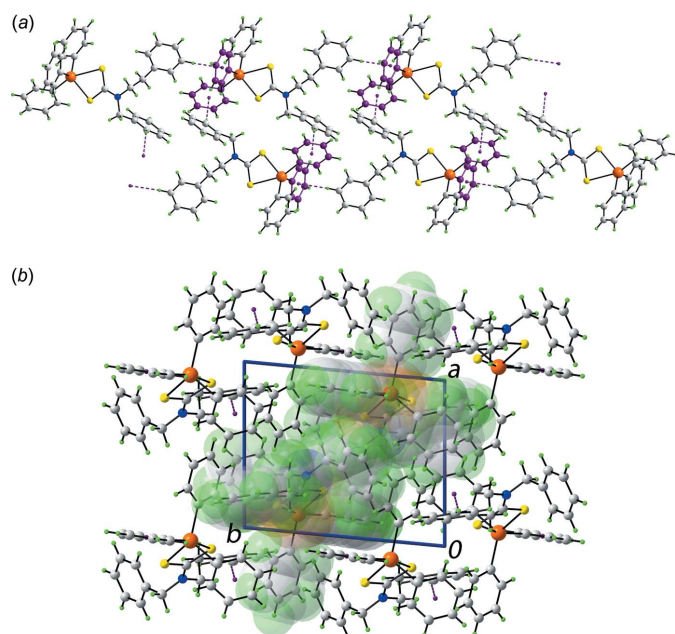


Figure 3

The molecular packing in (I): (a) supramolecular chain along the  $c$  axis sustained by dithiocarbamate-phenyl-C–H··· $\pi$ (Sn-phenyl) interactions shown as purple dashed lines and (b) a view of the unit-cell contents in projection down the  $c$  axis. In (a), the accepting rings are highlighted in purple and in (b), one chain is highlighted in space-filling mode.

Table 3

Hydrogen-bond geometry (Å, °) for (II).

$Cg1$  and  $Cg2$  are the centroids of the C8–C13 and C14–C19 rings, respectively.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C7-H7C \cdots Cg1^i$	0.98	2.94	3.821 (3)	151
$C13-H13 \cdots Cg2^{ii}$	0.95	2.98	3.7979 (18)	145
$C23-H23 \cdots Cg2^{iii}$	0.95	2.97	3.707 (2)	136

Symmetry codes: (i)  $-x, -y + 1, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 2$ ; (iii)  $x + 1, y, z$ .

phenyl ring with the result that a supramolecular chain is formed along the  $c$ -axis direction, Table 2 and Fig. 3a. The chains pack without directional interactions between them, Fig. 3b.

Even though there are oxygen atoms in the molecule of (II), the supramolecular association is dominated by C–H··· $\pi$  contacts involving methyl-C–H and Sn-bound-phenyl-C–H as donors and only two of the Sn-bound phenyl rings as acceptors, as the (C14–C19) ring accepts two interactions, Table 3. The result of this association is the formation of supramolecular layers in the  $ac$  plane, Fig. 4a. The layers stack along the  $b$  axis without directional interactions between them, Fig. 4b.

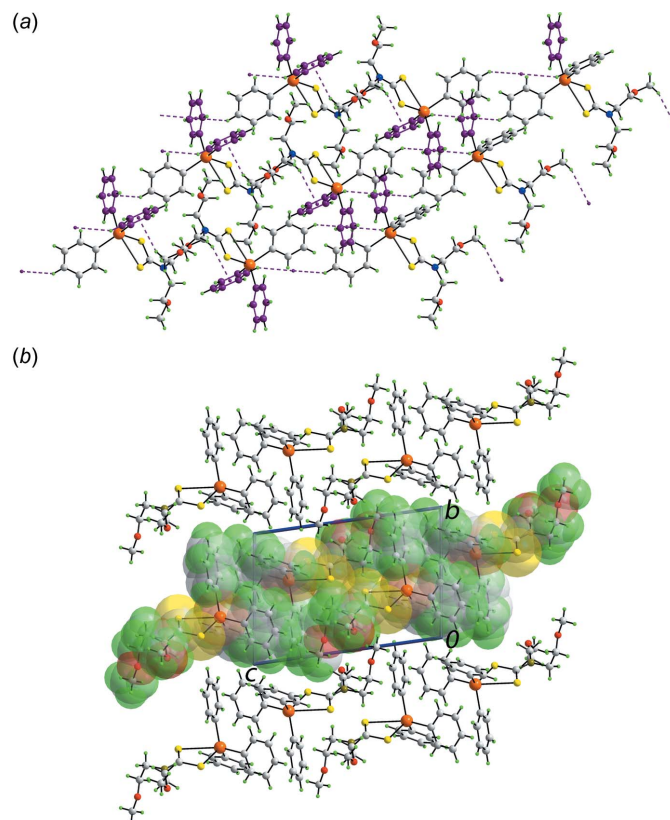
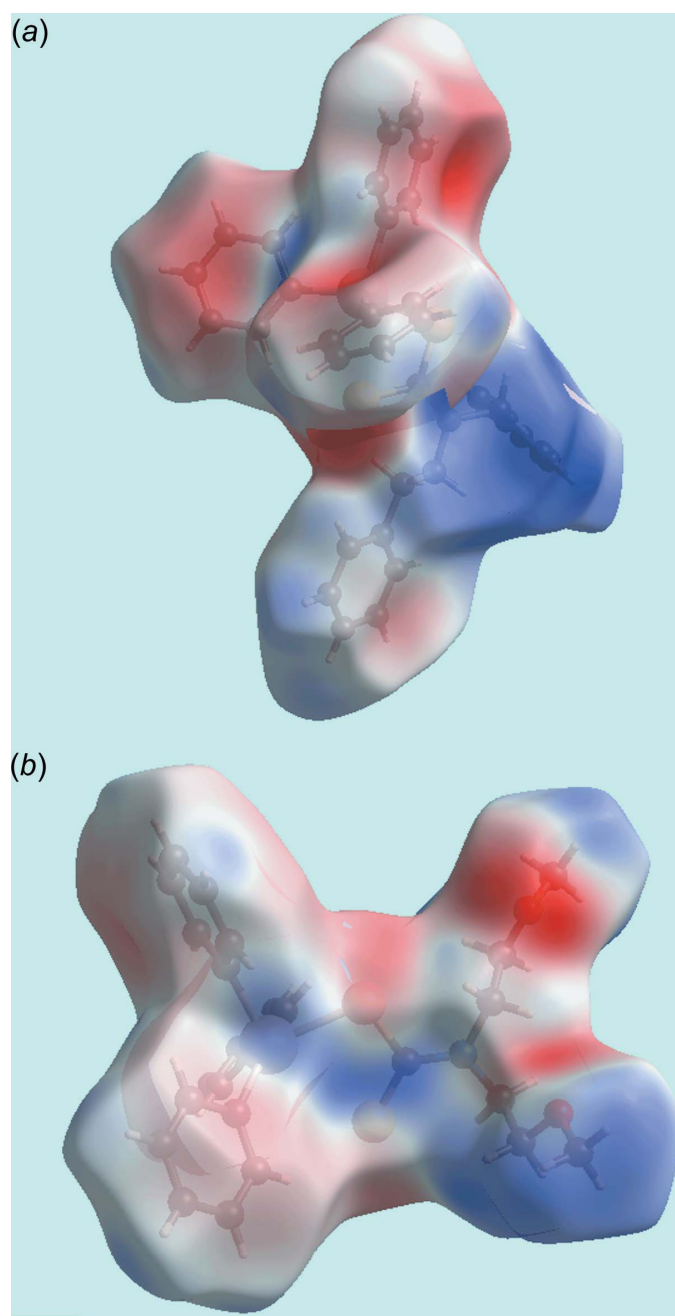


Figure 4

The molecular packing in (II): (a) supramolecular layer parallel to the  $ac$  plane sustained by methyl- and Sn-phenyl-C–H··· $\pi$ (Sn-phenyl) interactions shown as purple dashed lines and (b) a view of the unit-cell contents in projection down the  $a$  axis. In (a), the accepting rings are highlighted in purple and in (b), one layer is highlighted in space-filling mode.

### 3. Hirshfeld surface analysis

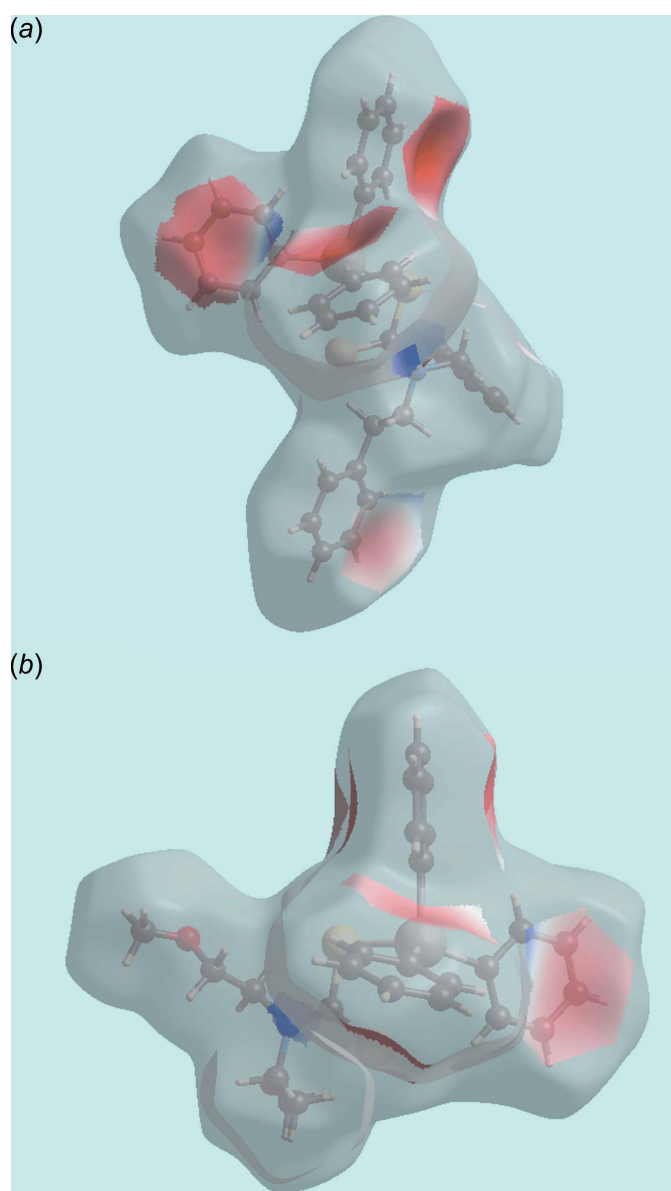
*Crystal Explorer* (Wolff *et al.*, 2012) was used to generate Hirshfeld surfaces mapped over  $d_{\text{norm}}$ , shape-index and electrostatic potential. The electrostatic potentials were calculated using *TONTO* (Spackman *et al.*, 2008; Jayatilaka *et al.*, 2005) integrated into *Crystal Explorer*, wherein the respective experimental structure was used as the input to *TONTO*. Further, the electrostatic potentials were mapped on Hirshfeld surfaces using the STO-3G basis set at the Hartree–Fock level of theory over ranges  $\pm 0.037$  au. and  $\pm 0.048$  au. for (I) and (II), respectively. The contact distances  $d_i$  and  $d_e$  from the



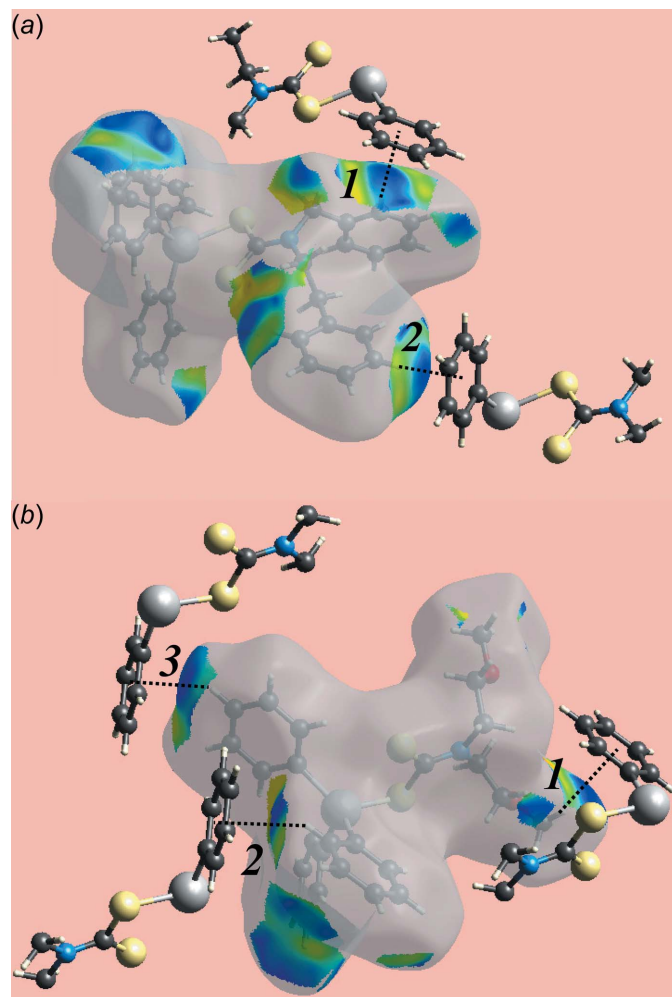
**Figure 5**  
Views of the Hirshfeld surfaces mapped over electrostatic potential (the red and blue regions represent negative and positive electrostatic potentials, respectively): (a) for (I) and (b) for (II).

Hirshfeld surface to the nearest atom inside and outside, respectively, enable the analysis of the intermolecular interactions through the mapping of  $d_{\text{norm}}$ . The combination of  $d_e$  and  $d_i$  in the form of two-dimensional fingerprint plots (McKinnon *et al.*, 2007) provides a useful summary of intermolecular contacts in the respective crystal.

The different shapes of Hirshfeld surfaces for molecules (I) and (II) arise from the asymmetric geometries resulting from the different dithiocarbamate-bound functional groups, *i.e.* phenyl and methoxy groups in (I) and (II), respectively, Fig. 5. The images of the Hirshfeld surface mapped over electrostatic potential for (I) and (II) display dark-red and dark-blue regions, assigned to negative and positive potentials, respectively, and are localized near their respective functional



**Figure 6**  
Views of Hirshfeld surfaces mapped over electrostatic potential corresponding to C...H contacts (the red spots located near the phenyl rings indicate their contribution as  $\pi$ -bond donors in the C–H... $\pi$  interactions) for: (a) (I) and (b) (II).



**Figure 7**  
Views of Hirshfeld surfaces mapped over shape-index (a) for (I) and (b) for (II). The different C–H··· $\pi$  contacts are labelled and indicated as dashed lines.

groups. The absence of conventional hydrogen bonds in the crystals of (I) and (II) is consistent with the non-appearance of characteristic red-spots in the Hirshfeld surface mapped over  $d_{\text{norm}}$  (not shown). The curvature of the Hirshfeld surfaces around the phenyl rings participating as acceptors in the C–H··· $\pi$  contacts determine the strength of these interactions in the crystal packing. In the structure of (I), the surfaces around the Sn-bound phenyl (C17–C22) and (C23–C28) rings are more concave than the equivalent rings participating in C–H··· $\pi$  interactions in (II), indicating their greater influence upon packing, as seen in the shorter H···ring centroid separations, Tables 2 and 3. This observation is also apparent from the Hirshfeld surfaces mapped over electrostatic potential corresponding to C···H contacts for (I) and (II), both showing red spots in the images of Fig. 6 correlating with their functioning as  $\pi$ -bond acceptors. The concave appearance of the Hirshfeld surface mapped over electrostatic potential around the Sn-bound phenyl ring (C14–C19) in the structure of (II) is indicative of its participation in two C–H··· $\pi$  interactions, *i.e.* with the H13 and H23 hydrogen atoms. The other C–H··· $\pi$  contact involves methyl-H7C atom as the

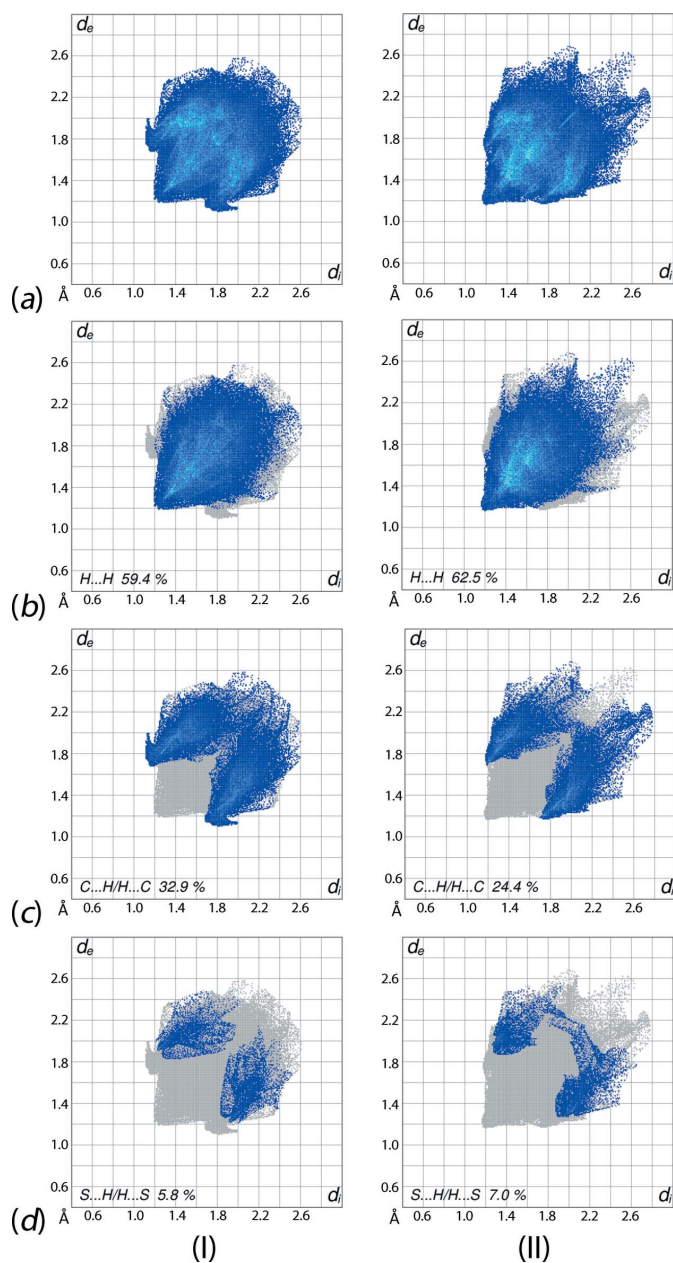
**Table 4**

Percentage contribution to interatomic contacts from the Hirshfeld surface for (I) and (II).

Contact	(I)	(II)
H···H	59.4	62.5
C···H/H···C	32.9	24.4
O···H/H···O	–	4.7
S···H/H···S	5.8	7.0
C···S/S···C	0.4	0.0
N···H/H···N	0.5	0.4
C···C	0.9	0.0
S···S	0.0	0.4
C···O/O···C	0.1	0.1
O···O	–	0.5

donor and phenyl (C8–C13) ring as the acceptor. The shape-indexed Hirshfeld surfaces highlighting the C–H··· $\pi$  contacts are shown in Fig. 7.

The overall two-dimensional fingerprint plots for (I) and (II) and those delineated into H···H, C···H/H···C and S···H/H···S contacts (McKinnon *et al.*, 2007) are illustrated in Fig. 8*a–d*, respectively; their relative contributions are summarized in Table 4. Although the distribution of points in the overall plots of (I) and (II) have almost same ( $d_e$ ,  $d_i$ ) ranges, *i.e.* between 1.2 and 2.6 Å, the densities and the areas of their distributions are different. It is evident from the data in Table 4 and the fingerprint plot delineated into H···H contacts in Fig. 8*b* that these contacts make the most significant contribution to the Hirshfeld surfaces of both (I) and (II). In the fingerprint plot of (I) delineated into H···H contacts (Fig. 8*b*), all the points are situated at the ( $d_e$ ,  $d_i$ ) distances greater than or equal to their van der Waals separations *i.e.*  $2 \times 1.2$  Å, hence there is no propensity to form such intermolecular contacts. The peak at ( $d_e$ ,  $d_i$ ) distances slightly less than van der Waals separations in the fingerprint plot for (II) is due to a short interatomic H···H contact between symmetry-related methoxy- and dithiocarbamate hydrogen atoms [H7A···H5A<sup>i</sup> = 2.36 Å; symmetry code: (i)  $-x, 2 - y, 1 - z$ ]. In the fingerprint plot delineated into C···H/H···C contacts for (I), Fig. 8*c*, the 32.9% contribution to the Hirshfeld surface and the symmetrical distribution of points showing bending of the pattern at ( $d_e + d_i$ )<sub>min</sub>  $\sim 2.8$  Å is the result of short interatomic C···H/H···C contacts [C1···H32<sup>ii</sup> = 2.85 and C14···H27<sup>iii</sup> = 2.84 Å; symmetry codes: (ii)  $1 + x, y, z$ ; (iii)  $1 - x, 2 - y, -z$ ]. In the structure of (II), a comparatively reduced contribution from these contacts to the surface is made, *i.e.* 24.4%, an observation ascribed to the presence of only C–H··· $\pi$  contacts in the molecular packing, with no other short inter-atomic contacts. The negligible contribution from C···C contacts to the Hirshfeld surfaces indicate that despite the presence of three Sn-bound phenyl rings in the structures of both (I) and (II), and the presence of other two phenyl rings bound to the dithiocarbamate ligand in (I), the structures show no significant  $\pi$ – $\pi$  stacking. In the structure of (II), the presence of oxygen atoms does not have any significant influence on its molecular packing although there is 4.7% contribution from O···H/H···O contacts to the Hirshfeld surface. The fingerprint plots delineated into S···H/H···S


**Figure 8**

Comparison between (I) and (II) of the (a) full two-dimensional fingerprint plots, and the plots delineated into (b) H...H, (c) C...H/H...C and (d) S...H/H...S contacts.

contacts for both the molecules (I) and (II), Fig. 8d, show that crowded geometries around the tin atoms prevent the sulfur atoms from forming such intermolecular contacts although these contacts have significant contributions to their respective Hirshfeld surfaces, Table 4, as well as nearly symmetrical distributions of points in their plots. This observation was also noted in an earlier study describing related organotin dithiocarbamate structures (Mohamad *et al.*, 2016).

#### 4. Database survey

According to a search of the Cambridge Structural Database (CSD; Groom *et al.*, 2016), the dithiocarbamate ligands

featuring in the present study have comparatively rare *R/R'* substituents. For example, the  $^-S_2CN(\text{Ben})CH_2CH_2Ph$  anion in (I) has only one precedent, namely in  $Pb[S_2CN(\text{Ben})CH_2CH_2Ph]_2$  (Sathiyaraj *et al.*, 2012). There are eight examples of the  $^-S_2CN(CH_2CH_2OMe)_2$  anion, as in (II), being the focus of two recent systematic studies (Hogarth *et al.*, 2009; Naeem *et al.*, 2010).

Reflecting the interest in organotin dithiocarbamates, there are approximately 40 examples of triphenyltin dithiocarbamate structures in the CSD, all of which present the same basic structural motif as described herein for (I) and (II). The prototype compound,  $Ph_3Sn(S_2CNEt_2)$  features the shortest Sn–S bond length of the series at 2.429 (3) Å (Hook *et al.*, 1994). The most asymmetric mode of coordination of a dithiocarbamate ligand, *i.e.* with  $\Delta(\text{Sn}–\text{S})$  of 0.74 Å, is found in the structure of  $Ph_3Sn(4\text{-nitrophenylpiperazine-1-dithiocarbamate})$  (Rehman *et al.*, 2009). On the other hand, the most symmetric mode of coordination is found in the structure of  $Ph_3Sn(4\text{-methoxyphenylpiperazine-1-dithiocarbamate})$ , having  $\Delta(\text{Sn}–\text{S})$  of 0.42 Å (Zia-ur-Rehman *et al.*, 2011), *i.e.* the same value as found in the structure of (I) reported herein.

#### 5. Synthesis and crystallization

**Synthesis of (I):** *N*-Benzyl-2-phenylethylamine (2 mmol) dissolved in ethanol (10 ml) was stirred for 30 min in an ice-bath. 25% ammonia (1–2 ml) was added to generate a basic solution. After that, a cold ethanolic solution of carbon disulfide (2 mmol) was added to the solution followed by stirring for about 2 h. Then, triphenyltin(IV) chloride (2 mmol) dissolved in ethanol (30 ml) was added drop wise into the solution followed by further stirring for 2 h. The precipitate that formed was filtered off and washed with cold ethanol a few times to remove impurities. Finally, the precipitate was dried in a desiccator. Recrystallization was achieved by dissolving the compound in a chloroform and ethanol mixture (1:1 v/v): this solution was allowed to slowly evaporate at room temperature yielding colourless slabs of (I). M.p.: 419–421 K. Yield: 85%. Analysis: found C, 64.5; H, 5.3; N, 2.3; S, 9.9.  $C_{34}H_{31}NS_2Sn$  requires: C, 64.2; H, 4.9; N, 2.2; S, 10.1. IR ( $cm^{-1}$ ): 1476  $\nu(\text{C}–\text{N})$ , 1021  $\nu(\text{C}–\text{S})$ , 502  $\nu(\text{Sn}–\text{C})$ , 448  $\nu(\text{Sn}–\text{S})$ .  $^1H$  NMR ( $CDCl_3$ ): 7.44–7.86 (15H, Sn–Ph), 7.16–7.39 (10H, C–Ph), 5.03 (2H,  $CH_2\text{Ben}$ ), 3.96 (2H,  $NCH_2CH_2$ ), 3.04 (2H,  $NCH_2CH_2$ ).  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ ):  $\delta$  197.8 ( $S_2C$ ), 126.7–142.3 (Ar), 59.8 ( $CH_2\text{Ben}$ ), 56.4 ( $NCH_2CH_2$ ), 32.8 ( $NCH_2CH_2$ ).  $^{119}Sn\{^1H\}$  NMR ( $CDCl_3$ ): –180.2.

Compound (II) was prepared in essentially the same manner as for (I) but using bis(2-methoxyethyl)amine (5 mmol) in place of *N*-benzyl-2-phenylethylamine. Recrystallization was from chloroform solution to yield colourless slabs. M.p.: 366–367 K. Yield: 89%. Analysis: found C, 54.4; H, 4.4; N, 2.9; S, 12.1.  $C_{25}H_{29}NO_2S_2Sn$  requires: C, 53.8; H, 5.2; N, 2.5; S, 11.5. IR ( $cm^{-1}$ ): 1470  $\nu(\text{C}–\text{N})$ , 994  $\nu(\text{C}–\text{S})$ , 559  $\nu(\text{Sn}–\text{C})$ , 425  $\nu(\text{Sn}–\text{S})$ .  $^1H$  NMR ( $CDCl_3$ ): 7.40–7.74 (15H, Sn–Ph), 4.13 (2H,  $OCH_2$ ), 3.72 (2H,  $NCH_2$ ), 3.35 (3H,  $CH_3$ ).  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ ):  $\delta$  197.3 ( $S_2C$ ), 128.6–142.4 (Ar), 70.0 ( $OCH_2$ ), 59.0 ( $NCH_2$ ), 57.1 ( $CH_3$ ).  $^{119}Sn\{^1H\}$  NMR ( $CDCl_3$ ): –185.0.

**Table 5**  
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	[Sn(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> (C <sub>16</sub> H <sub>16</sub> NS <sub>2</sub> )]	[Sn(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> (C <sub>7</sub> H <sub>14</sub> NO <sub>2</sub> S <sub>2</sub> )]
<i>M<sub>r</sub></i>	636.41	558.35
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	139	147
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.5856 (2), 11.6140 (2), 13.6795 (3)	9.6703 (2), 9.8015 (2), 13.8515 (3)
$\alpha$ , $\beta$ , $\gamma$ (°)	78.043 (2), 77.868 (2), 82.358 (2)	95.092 (2), 99.467 (2), 105.841 (2)
<i>V</i> (Å <sup>3</sup> )	1450.20 (5)	1233.41 (5)
<i>Z</i>	2	2
Radiation type	Mo <i>K</i> $\alpha$	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.05	1.23
Crystal size (mm)	0.50 × 0.30 × 0.20	0.50 × 0.50 × 0.20
Data collection		
Diffractometer	Agilent Technologies SuperNova Dual diffractometer with an Atlas detector	Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Agilent, 2015)	Multi-scan ( <i>CrysAlis PRO</i> ; Agilent, 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.804, 1.000	0.722, 1.000
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	41508, 9103, 8428	35286, 7773, 7157
<i>R<sub>int</sub></i>	0.038	0.035
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.741	0.740
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.022, 0.055, 1.00	0.023, 0.056, 1.03
No. of reflections	9103	7773
No. of parameters	343	290
No. of restraints	0	18
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.53, -0.61	0.55, -0.61

Computer programs: *CrysAlis PRO* (Agilent, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *pubCIF* (Westrip, 2010).

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. Carbon-bound H atoms were placed in calculated positions (C–H = 0.95–0.99 Å) and were included in the refinement in the riding-model approximation, with *U*<sub>iso</sub>(H) set to 1.2–1.5*U*<sub>eq</sub>(C). In the refinement of (II), disorder was noted in the C5-chain of the dithiocarbamate ligand. Specifically, the C6 and O2 atoms were modelled over two positions in the ratio 0.569 (2):0.431 (2). The anisotropic displacement parameters for both components of the C6 and O5 atoms were constrained to be equivalent; further, those for the C6 atoms were restrained to be approximately isotropic. The 1,2 and 1,3 bond lengths of the disordered residual were restrained to be similar to those of the ordered arm of the dithiocarbamate ligand.

## Acknowledgements

This work was supported by grant FRGS/2/2013/SKK10/UKM/02/1. We gratefully acknowledge the School of Chemical Science and Food Technology, Universiti Kebangsaan Malaysia, for providing the essential laboratory facilities. We would also like to thank the laboratory assistants of the Faculty of Science and Technology, Universiti Kebangsaan Malaysia for technical support. Intensity data were collected in the University of Malaya's Crystallographic Laboratory.

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## supporting information

*Acta Cryst.* (2016). E72, 1480-1487 [doi:10.1107/S2056989016014985]

## [*N*-Benzyl-*N*-(2-phenylethyl)dithiocarbamato- $\kappa^2$ S,S']triphenyltin(IV) and [bis(2-methoxyethyl)dithiocarbamato- $\kappa^2$ S,S']triphenyltin(IV): crystal structures and Hirshfeld surface analysis

Rapidah Mohamad, Normah Awang, Nurul Farahana Kamaludin, Mukesh M. Jotani and Edward R. T. Tiekink

### Computing details

For both compounds, data collection: *CrysAlis PRO* (Agilent, 2015); cell refinement: *CrysAlis PRO* (Agilent, 2015); data reduction: *CrysAlis PRO* (Agilent, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### (I) [*N*-Benzyl-*N*-(2-phenylethyl)dithiocarbamato- $\kappa^2$ S,S']triphenyltin(IV)

#### Crystal data

[Sn(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>(C<sub>16</sub>H<sub>16</sub>NS<sub>2</sub>)]

$M_r = 636.41$

Triclinic,  $P\bar{1}$

$a = 9.5856$  (2) Å

$b = 11.6140$  (2) Å

$c = 13.6795$  (3) Å

$\alpha = 78.043$  (2)°

$\beta = 77.868$  (2)°

$\gamma = 82.358$  (2)°

$V = 1450.20$  (5) Å<sup>3</sup>

$Z = 2$

$F(000) = 648$

$D_x = 1.457$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 26203 reflections

$\theta = 4.1\text{--}31.4^\circ$

$\mu = 1.05$  mm<sup>-1</sup>

$T = 139$  K

Slab, colourless

$0.50 \times 0.30 \times 0.20$  mm

#### Data collection

Agilent Technologies SuperNova Dual  
diffractometer with an Atlas detector  
Radiation source: SuperNova (Mo) X-ray  
Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  scan

Absorption correction: multi-scan  
(*CrysAlis PRO*; Agilent, 2015)

$T_{\min} = 0.804$ ,  $T_{\max} = 1.000$

41508 measured reflections

9103 independent reflections

8428 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 31.8^\circ$ ,  $\theta_{\min} = 3.3^\circ$

$h = -13 \rightarrow 14$

$k = -17 \rightarrow 17$

$l = -19 \rightarrow 19$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.055$

$S = 1.00$

9103 reflections

343 parameters

0 restraints

Hydrogen site location: inferred from  
neighbouring sites  
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 0.5974P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.003$   
 $\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.61 \text{ e } \text{\AA}^{-3}$

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn	0.11097 (2)	0.73083 (2)	-0.11080 (2)	0.01757 (3)
S1	0.26398 (4)	0.60268 (3)	0.00262 (3)	0.02307 (7)
S2	0.14838 (4)	0.83511 (3)	0.05703 (3)	0.02241 (7)
N1	0.34474 (13)	0.69202 (11)	0.14450 (9)	0.0226 (2)
C1	0.25975 (14)	0.71037 (11)	0.07630 (10)	0.0195 (2)
C2	0.45063 (16)	0.58852 (14)	0.15813 (11)	0.0276 (3)
H2A	0.5464	0.6161	0.1504	0.033*
H2B	0.4549	0.5425	0.1040	0.033*
C3	0.41603 (15)	0.50885 (13)	0.26046 (11)	0.0242 (3)
C4	0.51461 (16)	0.48312 (14)	0.32492 (12)	0.0299 (3)
H4	0.6025	0.5186	0.3057	0.036*
C5	0.48559 (19)	0.40590 (17)	0.41719 (13)	0.0383 (4)
H5	0.5538	0.3884	0.4607	0.046*
C6	0.3580 (2)	0.35456 (16)	0.44587 (14)	0.0402 (4)
H6	0.3389	0.3007	0.5086	0.048*
C7	0.25767 (19)	0.38180 (15)	0.38302 (15)	0.0390 (4)
H7	0.1689	0.3477	0.4033	0.047*
C8	0.28613 (17)	0.45813 (14)	0.29129 (13)	0.0317 (3)
H8	0.2167	0.4764	0.2486	0.038*
C9	0.34155 (15)	0.78002 (13)	0.20882 (11)	0.0252 (3)
H9A	0.3358	0.8602	0.1667	0.030*
H9B	0.4319	0.7680	0.2353	0.030*
C10	0.21466 (18)	0.77186 (14)	0.29854 (11)	0.0293 (3)
H10A	0.1252	0.7726	0.2731	0.035*
H10B	0.2276	0.6961	0.3461	0.035*
C11	0.20107 (15)	0.87303 (13)	0.35476 (10)	0.0226 (3)
C12	0.22314 (16)	0.85318 (14)	0.45412 (11)	0.0268 (3)
H12	0.2495	0.7751	0.4866	0.032*
C13	0.20723 (17)	0.94591 (15)	0.50684 (11)	0.0298 (3)
H13	0.2219	0.9310	0.5751	0.036*
C14	0.17019 (17)	1.05948 (14)	0.45984 (12)	0.0309 (3)
H14	0.1583	1.1229	0.4958	0.037*
C15	0.15027 (17)	1.08086 (14)	0.35992 (13)	0.0306 (3)
H15	0.1260	1.1593	0.3272	0.037*

C16	0.16559 (16)	0.98869 (14)	0.30788 (11)	0.0273 (3)
H16	0.1518	1.0042	0.2394	0.033*
C17	0.11990 (14)	0.59670 (12)	-0.20181 (10)	0.0202 (2)
C18	0.12215 (15)	0.62884 (12)	-0.30614 (11)	0.0226 (3)
H18	0.1261	0.7095	-0.3379	0.027*
C19	0.11864 (16)	0.54453 (14)	-0.36467 (12)	0.0280 (3)
H19	0.1215	0.5677	-0.4358	0.034*
C20	0.11097 (17)	0.42673 (14)	-0.31871 (13)	0.0318 (3)
H20	0.1072	0.3693	-0.3582	0.038*
C21	0.10880 (17)	0.39296 (13)	-0.21536 (13)	0.0317 (3)
H21	0.1038	0.3122	-0.1840	0.038*
C22	0.11387 (15)	0.47709 (12)	-0.15718 (11)	0.0253 (3)
H22	0.1132	0.4530	-0.0864	0.030*
C23	0.23372 (14)	0.86620 (12)	-0.20545 (10)	0.0196 (2)
C24	0.18559 (18)	0.98566 (13)	-0.21328 (12)	0.0290 (3)
H24	0.0933	1.0088	-0.1776	0.035*
C25	0.2715 (2)	1.07114 (15)	-0.27286 (14)	0.0412 (4)
H25	0.2374	1.1524	-0.2779	0.049*
C26	0.4055 (2)	1.03887 (18)	-0.32465 (14)	0.0444 (4)
H26	0.4642	1.0977	-0.3648	0.053*
C27	0.45457 (18)	0.92100 (19)	-0.31816 (15)	0.0434 (4)
H27	0.5470	0.8986	-0.3541	0.052*
C28	0.36913 (15)	0.83497 (15)	-0.25919 (12)	0.0306 (3)
H28	0.4034	0.7539	-0.2554	0.037*
C29	-0.11619 (14)	0.77083 (11)	-0.06779 (10)	0.0194 (2)
C30	-0.18103 (15)	0.85380 (12)	-0.00804 (12)	0.0256 (3)
H30	-0.1239	0.8910	0.0229	0.031*
C31	-0.32861 (16)	0.88286 (14)	0.00684 (13)	0.0320 (3)
H31	-0.3716	0.9393	0.0482	0.038*
C32	-0.41312 (16)	0.82989 (14)	-0.03838 (13)	0.0318 (3)
H32	-0.5136	0.8511	-0.0293	0.038*
C33	-0.35052 (16)	0.74601 (14)	-0.09672 (13)	0.0318 (3)
H33	-0.4082	0.7085	-0.1270	0.038*
C34	-0.20313 (15)	0.71655 (13)	-0.11116 (12)	0.0256 (3)
H34	-0.1610	0.6586	-0.1511	0.031*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn	0.01871 (5)	0.01729 (5)	0.01588 (4)	-0.00169 (3)	-0.00165 (3)	-0.00279 (3)
S1	0.02930 (17)	0.01917 (15)	0.02176 (15)	0.00255 (12)	-0.00751 (13)	-0.00641 (12)
S2	0.02570 (16)	0.02023 (15)	0.02146 (15)	0.00247 (12)	-0.00597 (13)	-0.00562 (12)
N1	0.0248 (5)	0.0254 (6)	0.0181 (5)	0.0031 (4)	-0.0055 (4)	-0.0067 (4)
C1	0.0213 (6)	0.0199 (6)	0.0164 (6)	-0.0022 (5)	-0.0008 (5)	-0.0034 (5)
C2	0.0258 (7)	0.0334 (8)	0.0221 (7)	0.0085 (6)	-0.0061 (5)	-0.0070 (6)
C3	0.0267 (7)	0.0236 (6)	0.0234 (6)	0.0049 (5)	-0.0075 (5)	-0.0085 (5)
C4	0.0242 (7)	0.0363 (8)	0.0281 (7)	0.0037 (6)	-0.0081 (6)	-0.0044 (6)
C5	0.0348 (8)	0.0473 (10)	0.0287 (8)	0.0094 (7)	-0.0119 (7)	-0.0003 (7)

C6	0.0443 (9)	0.0324 (8)	0.0345 (9)	0.0058 (7)	-0.0027 (7)	0.0039 (7)
C7	0.0360 (8)	0.0285 (8)	0.0507 (11)	-0.0051 (6)	-0.0076 (8)	-0.0026 (7)
C8	0.0331 (8)	0.0281 (7)	0.0384 (9)	-0.0019 (6)	-0.0158 (7)	-0.0078 (7)
C9	0.0276 (7)	0.0302 (7)	0.0204 (6)	-0.0024 (5)	-0.0055 (5)	-0.0095 (6)
C10	0.0392 (8)	0.0292 (7)	0.0190 (6)	-0.0071 (6)	0.0008 (6)	-0.0075 (6)
C11	0.0238 (6)	0.0262 (7)	0.0173 (6)	-0.0025 (5)	-0.0016 (5)	-0.0050 (5)
C12	0.0318 (7)	0.0289 (7)	0.0173 (6)	-0.0015 (6)	-0.0034 (5)	-0.0012 (5)
C13	0.0329 (8)	0.0406 (8)	0.0177 (6)	-0.0091 (6)	-0.0030 (6)	-0.0078 (6)
C14	0.0316 (7)	0.0323 (8)	0.0296 (8)	-0.0094 (6)	0.0037 (6)	-0.0132 (6)
C15	0.0322 (7)	0.0253 (7)	0.0315 (8)	-0.0013 (6)	-0.0025 (6)	-0.0032 (6)
C16	0.0313 (7)	0.0309 (7)	0.0191 (6)	-0.0008 (6)	-0.0079 (5)	-0.0014 (5)
C17	0.0188 (6)	0.0201 (6)	0.0204 (6)	-0.0017 (4)	-0.0007 (5)	-0.0043 (5)
C18	0.0247 (6)	0.0219 (6)	0.0214 (6)	-0.0005 (5)	-0.0059 (5)	-0.0043 (5)
C19	0.0280 (7)	0.0350 (8)	0.0239 (7)	-0.0028 (6)	-0.0057 (6)	-0.0111 (6)
C20	0.0306 (7)	0.0329 (8)	0.0358 (8)	-0.0073 (6)	-0.0007 (6)	-0.0184 (7)
C21	0.0368 (8)	0.0213 (7)	0.0355 (8)	-0.0087 (6)	0.0034 (7)	-0.0082 (6)
C22	0.0291 (7)	0.0224 (6)	0.0219 (6)	-0.0052 (5)	0.0018 (5)	-0.0037 (5)
C23	0.0213 (6)	0.0220 (6)	0.0163 (6)	-0.0052 (5)	-0.0045 (5)	-0.0026 (5)
C24	0.0401 (8)	0.0226 (7)	0.0235 (7)	-0.0042 (6)	-0.0003 (6)	-0.0072 (6)
C25	0.0680 (12)	0.0241 (7)	0.0330 (9)	-0.0168 (8)	-0.0050 (8)	-0.0051 (7)
C26	0.0520 (11)	0.0491 (11)	0.0348 (9)	-0.0343 (9)	-0.0072 (8)	0.0039 (8)
C27	0.0230 (7)	0.0605 (12)	0.0408 (10)	-0.0135 (7)	-0.0005 (7)	0.0044 (9)
C28	0.0207 (6)	0.0349 (8)	0.0315 (8)	-0.0002 (6)	-0.0023 (6)	0.0003 (6)
C29	0.0196 (6)	0.0180 (6)	0.0180 (6)	-0.0014 (4)	-0.0014 (5)	0.0003 (5)
C30	0.0249 (6)	0.0223 (6)	0.0288 (7)	0.0006 (5)	-0.0033 (5)	-0.0065 (6)
C31	0.0257 (7)	0.0266 (7)	0.0391 (9)	0.0043 (6)	0.0012 (6)	-0.0073 (6)
C32	0.0194 (6)	0.0285 (7)	0.0411 (9)	0.0002 (5)	-0.0004 (6)	0.0013 (6)
C33	0.0235 (7)	0.0336 (8)	0.0392 (9)	-0.0053 (6)	-0.0079 (6)	-0.0050 (7)
C34	0.0236 (6)	0.0255 (7)	0.0276 (7)	-0.0026 (5)	-0.0039 (5)	-0.0055 (6)

*Geometric parameters (Å, °)*

Sn—C23	2.1309 (13)	C14—H14	0.9500
Sn—C29	2.1469 (13)	C15—C16	1.380 (2)
Sn—C17	2.1696 (13)	C15—H15	0.9500
Sn—S1	2.4886 (4)	C16—H16	0.9500
Sn—S2	2.9120 (3)	C17—C18	1.3947 (19)
S1—C1	1.7532 (13)	C17—C22	1.4003 (19)
S2—C1	1.6902 (13)	C18—C19	1.3949 (19)
N1—C1	1.3305 (18)	C18—H18	0.9500
N1—C9	1.4739 (17)	C19—C20	1.387 (2)
N1—C2	1.4739 (17)	C19—H19	0.9500
C2—C3	1.508 (2)	C20—C21	1.383 (2)
C2—H2A	0.9900	C20—H20	0.9500
C2—H2B	0.9900	C21—C22	1.393 (2)
C3—C4	1.388 (2)	C21—H21	0.9500
C3—C8	1.395 (2)	C22—H22	0.9500
C4—C5	1.387 (2)	C23—C24	1.3922 (19)

C4—H4	0.9500	C23—C28	1.3932 (19)
C5—C6	1.379 (3)	C24—C25	1.388 (2)
C5—H5	0.9500	C24—H24	0.9500
C6—C7	1.385 (3)	C25—C26	1.376 (3)
C6—H6	0.9500	C25—H25	0.9500
C7—C8	1.376 (2)	C26—C27	1.378 (3)
C7—H7	0.9500	C26—H26	0.9500
C8—H8	0.9500	C27—C28	1.388 (2)
C9—C10	1.533 (2)	C27—H27	0.9500
C9—H9A	0.9900	C28—H28	0.9500
C9—H9B	0.9900	C29—C30	1.3915 (18)
C10—C11	1.5102 (19)	C29—C34	1.3952 (19)
C10—H10A	0.9900	C30—C31	1.392 (2)
C10—H10B	0.9900	C30—H30	0.9500
C11—C12	1.3869 (19)	C31—C32	1.385 (2)
C11—C16	1.394 (2)	C31—H31	0.9500
C12—C13	1.391 (2)	C32—C33	1.383 (2)
C12—H12	0.9500	C32—H32	0.9500
C13—C14	1.378 (2)	C33—C34	1.391 (2)
C13—H13	0.9500	C33—H33	0.9500
C14—C15	1.387 (2)	C34—H34	0.9500
C23—Sn—C29	118.33 (5)	C13—C14—C15	119.82 (14)
C23—Sn—C17	106.09 (5)	C13—C14—H14	120.1
C29—Sn—C17	101.34 (5)	C15—C14—H14	120.1
C23—Sn—S1	108.24 (4)	C16—C15—C14	120.25 (15)
C29—Sn—S1	124.31 (4)	C16—C15—H15	119.9
C17—Sn—S1	92.98 (4)	C14—C15—H15	119.9
C23—Sn—S2	85.28 (3)	C15—C16—C11	120.67 (14)
C29—Sn—S2	88.48 (4)	C15—C16—H16	119.7
C17—Sn—S2	158.55 (4)	C11—C16—H16	119.7
S1—Sn—S2	65.919 (10)	C18—C17—C22	118.10 (12)
C1—S1—Sn	93.73 (5)	C18—C17—Sn	120.38 (10)
C1—S2—Sn	81.22 (5)	C22—C17—Sn	121.39 (10)
C1—N1—C9	120.43 (11)	C17—C18—C19	121.14 (13)
C1—N1—C2	123.71 (11)	C17—C18—H18	119.4
C9—N1—C2	115.81 (11)	C19—C18—H18	119.4
N1—C1—S2	122.25 (10)	C20—C19—C18	119.81 (14)
N1—C1—S1	119.24 (10)	C20—C19—H19	120.1
S2—C1—S1	118.51 (8)	C18—C19—H19	120.1
N1—C2—C3	112.93 (11)	C21—C20—C19	119.96 (14)
N1—C2—H2A	109.0	C21—C20—H20	120.0
C3—C2—H2A	109.0	C19—C20—H20	120.0
N1—C2—H2B	109.0	C20—C21—C22	120.16 (14)
C3—C2—H2B	109.0	C20—C21—H21	119.9
H2A—C2—H2B	107.8	C22—C21—H21	119.9
C4—C3—C8	118.84 (15)	C21—C22—C17	120.82 (14)
C4—C3—C2	120.27 (14)	C21—C22—H22	119.6

C8—C3—C2	120.88 (13)	C17—C22—H22	119.6
C5—C4—C3	120.38 (15)	C24—C23—C28	118.41 (13)
C5—C4—H4	119.8	C24—C23—Sn	122.40 (10)
C3—C4—H4	119.8	C28—C23—Sn	119.16 (10)
C6—C5—C4	120.19 (16)	C23—C24—C25	120.47 (15)
C6—C5—H5	119.9	C23—C24—H24	119.8
C4—C5—H5	119.9	C25—C24—H24	119.8
C5—C6—C7	119.79 (17)	C26—C25—C24	120.40 (16)
C5—C6—H6	120.1	C26—C25—H25	119.8
C7—C6—H6	120.1	C24—C25—H25	119.8
C8—C7—C6	120.22 (17)	C25—C26—C27	119.89 (16)
C8—C7—H7	119.9	C25—C26—H26	120.1
C6—C7—H7	119.9	C27—C26—H26	120.1
C7—C8—C3	120.55 (15)	C28—C27—C26	120.08 (16)
C7—C8—H8	119.7	C28—C27—H27	120.0
C3—C8—H8	119.7	C26—C27—H27	120.0
N1—C9—C10	112.51 (12)	C27—C28—C23	120.74 (15)
N1—C9—H9A	109.1	C27—C28—H28	119.6
C10—C9—H9A	109.1	C23—C28—H28	119.6
N1—C9—H9B	109.1	C30—C29—C34	118.28 (12)
C10—C9—H9B	109.1	C30—C29—Sn	124.91 (10)
H9A—C9—H9B	107.8	C34—C29—Sn	116.54 (9)
C11—C10—C9	111.70 (12)	C31—C30—C29	120.74 (14)
C11—C10—H10A	109.3	C31—C30—H30	119.6
C9—C10—H10A	109.3	C29—C30—H30	119.6
C11—C10—H10B	109.3	C30—C31—C32	120.27 (14)
C9—C10—H10B	109.3	C30—C31—H31	119.9
H10A—C10—H10B	107.9	C32—C31—H31	119.9
C12—C11—C16	118.47 (13)	C33—C32—C31	119.65 (14)
C12—C11—C10	120.88 (13)	C33—C32—H32	120.2
C16—C11—C10	120.65 (13)	C31—C32—H32	120.2
C11—C12—C13	120.94 (14)	C32—C33—C34	120.05 (15)
C11—C12—H12	119.5	C32—C33—H33	120.0
C13—C12—H12	119.5	C34—C33—H33	120.0
C14—C13—C12	119.83 (14)	C33—C34—C29	120.98 (13)
C14—C13—H13	120.1	C33—C34—H34	119.5
C12—C13—H13	120.1	C29—C34—H34	119.5
C9—N1—C1—S2	1.80 (18)	C13—C14—C15—C16	0.8 (2)
C2—N1—C1—S2	-175.36 (11)	C14—C15—C16—C11	0.1 (2)
C9—N1—C1—S1	-178.87 (10)	C12—C11—C16—C15	-1.2 (2)
C2—N1—C1—S1	3.97 (19)	C10—C11—C16—C15	178.66 (14)
Sn—S2—C1—N1	172.23 (12)	C22—C17—C18—C19	-0.1 (2)
Sn—S2—C1—S1	-7.10 (7)	Sn—C17—C18—C19	-175.86 (10)
Sn—S1—C1—N1	-171.12 (11)	C17—C18—C19—C20	0.8 (2)
Sn—S1—C1—S2	8.24 (8)	C18—C19—C20—C21	-0.9 (2)
C1—N1—C2—C3	-114.69 (15)	C19—C20—C21—C22	0.2 (2)
C9—N1—C2—C3	68.04 (16)	C20—C21—C22—C17	0.6 (2)

N1—C2—C3—C4	-122.90 (15)	C18—C17—C22—C21	-0.6 (2)
N1—C2—C3—C8	58.25 (18)	Sn—C17—C22—C21	175.12 (11)
C8—C3—C4—C5	1.6 (2)	C28—C23—C24—C25	-0.4 (2)
C2—C3—C4—C5	-177.25 (14)	Sn—C23—C24—C25	177.51 (12)
C3—C4—C5—C6	-0.4 (3)	C23—C24—C25—C26	-0.2 (3)
C4—C5—C6—C7	-1.1 (3)	C24—C25—C26—C27	0.6 (3)
C5—C6—C7—C8	1.2 (3)	C25—C26—C27—C28	-0.2 (3)
C6—C7—C8—C3	0.1 (3)	C26—C27—C28—C23	-0.4 (3)
C4—C3—C8—C7	-1.5 (2)	C24—C23—C28—C27	0.7 (2)
C2—C3—C8—C7	177.40 (14)	Sn—C23—C28—C27	-177.25 (13)
C1—N1—C9—C10	79.44 (17)	C34—C29—C30—C31	-0.8 (2)
C2—N1—C9—C10	-103.19 (15)	Sn—C29—C30—C31	173.03 (12)
N1—C9—C10—C11	-171.97 (12)	C29—C30—C31—C32	-0.4 (2)
C9—C10—C11—C12	-113.86 (16)	C30—C31—C32—C33	1.4 (2)
C9—C10—C11—C16	66.32 (19)	C31—C32—C33—C34	-1.0 (2)
C16—C11—C12—C13	1.4 (2)	C32—C33—C34—C29	-0.2 (2)
C10—C11—C12—C13	-178.42 (14)	C30—C29—C34—C33	1.2 (2)
C11—C12—C13—C14	-0.5 (2)	Sn—C29—C34—C33	-173.21 (12)
C12—C13—C14—C15	-0.6 (2)		

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

Cg1 and Cg2 are the centroids of the C17–C22 and C23–C28 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 $\cdots$ Cg1 <sup>i</sup>	0.95	2.63	3.4732 (17)	148
C13—H13 $\cdots$ Cg2 <sup>ii</sup>	0.95	2.62	3.5227 (17)	159

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $x, y, z+1$ .

**(II) [Bis(2-methoxyethyl)dithiocarbamate- $\kappa^2S,S'$ ]triphenyltin(IV)***Crystal data*

$[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_7\text{H}_{14}\text{NO}_2\text{S}_2)]$

$M_r = 558.35$

Triclinic,  $P\bar{1}$

$a = 9.6703$  (2)  $\text{\AA}$

$b = 9.8015$  (2)  $\text{\AA}$

$c = 13.8515$  (3)  $\text{\AA}$

$\alpha = 95.092$  (2) $^\circ$

$\beta = 99.467$  (2) $^\circ$

$\gamma = 105.841$  (2) $^\circ$

$V = 1233.41$  (5)  $\text{\AA}^3$

$Z = 2$

$F(000) = 568$

$D_x = 1.503$   $\text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$   $\text{\AA}$

Cell parameters from 22178 reflections

$\theta = 3.5\text{--}31.4^\circ$

$\mu = 1.23$   $\text{mm}^{-1}$

$T = 147$  K

Slab, colourless

$0.50 \times 0.50 \times 0.20$  mm

*Data collection*

Agilent Technologies SuperNova Dual  
diffractometer with an Atlas detector  
Radiation source: SuperNova (Mo) X-ray  
Source

Mirror monochromator

Detector resolution: 10.4041 pixels  $\text{mm}^{-1}$

$\omega$  scan

Absorption correction: multi-scan  
(CrysAlis PRO; Agilent, 2015)

$T_{\min} = 0.722$ ,  $T_{\max} = 1.000$

35286 measured reflections

7773 independent reflections

7157 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 31.7^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -14 \rightarrow 14$

$k = -14 \rightarrow 14$   
 $l = -20 \rightarrow 20$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.056$   
 $S = 1.03$   
 7773 reflections  
 290 parameters  
 18 restraints

Hydrogen site location: inferred from neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0258P)^2 + 0.4182P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.55 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.61 \text{ e } \text{\AA}^{-3}$

### Special details

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

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn	0.39512 (2)	0.60246 (2)	0.81652 (2)	0.01772 (3)	
S1	0.25030 (4)	0.72645 (4)	0.71341 (3)	0.02167 (7)	
S2	0.40147 (5)	0.56965 (4)	0.59282 (3)	0.02642 (8)	
O1	0.32503 (13)	0.89169 (13)	0.37430 (9)	0.0305 (3)	
C1	0.28578 (16)	0.66905 (15)	0.59818 (10)	0.0193 (3)	
C2	0.23365 (17)	0.66021 (16)	0.41897 (11)	0.0232 (3)	
H2A	0.1416	0.6499	0.3716	0.028*	
H2B	0.2501	0.5648	0.4179	0.028*	
C3	0.35905 (18)	0.76178 (17)	0.38579 (12)	0.0260 (3)	
H3A	0.4505	0.7801	0.4356	0.031*	
H3B	0.3740	0.7191	0.3223	0.031*	
C4	0.4413 (2)	0.9955 (2)	0.34738 (15)	0.0396 (4)	
H4A	0.5295	1.0166	0.3991	0.059*	
H4B	0.4133	1.0834	0.3397	0.059*	
H4C	0.4612	0.9581	0.2848	0.059*	
N1	0.21672 (13)	0.70856 (13)	0.51881 (9)	0.0192 (2)	0.569 (2)
C5	0.12069 (19)	0.8002 (2)	0.52550 (12)	0.0312 (4)	0.569 (2)
H5A	0.1610	0.8662	0.5884	0.037*	0.569 (2)
H5B	0.1316	0.8599	0.4716	0.037*	0.569 (2)
C6	-0.0309 (3)	0.7431 (3)	0.5215 (2)	0.0246 (5)	0.569 (2)
H6A	-0.0480	0.6835	0.5749	0.030*	0.569 (2)
H6B	-0.0783	0.6824	0.4572	0.030*	0.569 (2)
O2	-0.0900 (2)	0.8591 (3)	0.53320 (18)	0.0365 (4)	0.569 (2)
C7	-0.2292 (3)	0.8147 (2)	0.50101 (19)	0.0547 (6)	0.569 (2)
H7A	-0.2693	0.8963	0.5028	0.082*	0.569 (2)
H7B	-0.2748	0.7471	0.5428	0.082*	0.569 (2)
H7C	-0.2499	0.7667	0.4329	0.082*	0.569 (2)
N1'	0.21672 (13)	0.70856 (13)	0.51881 (9)	0.0192 (2)	0.431 (2)



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C5'	0.12069 (19)	0.8002 (2)	0.52550 (12)	0.0312 (4)	0.431 (2)
H5C	0.1118	0.8508	0.4671	0.037*	0.431 (2)
H5D	0.1553	0.8710	0.5863	0.037*	0.431 (2)
C6'	-0.0389 (4)	0.6765 (4)	0.5286 (3)	0.0246 (5)	0.431 (2)
H6C	-0.0856	0.6263	0.4611	0.030*	0.431 (2)
H6D	-0.0192	0.6046	0.5706	0.030*	0.431 (2)
O2'	-0.1349 (3)	0.7437 (3)	0.5672 (2)	0.0365 (4)	0.431 (2)
C7'	-0.2292 (3)	0.8147 (2)	0.50101 (19)	0.0547 (6)	0.431 (2)
H7D	-0.1720	0.8653	0.4560	0.082*	0.431 (2)
H7E	-0.2602	0.8830	0.5422	0.082*	0.431 (2)
H7F	-0.3159	0.7412	0.4625	0.082*	0.431 (2)
C8	0.29263 (16)	0.37698 (15)	0.78961 (10)	0.0188 (3)	
C9	0.14085 (17)	0.32430 (17)	0.75699 (11)	0.0238 (3)	
H9	0.0851	0.3895	0.7456	0.029*	
C10	0.07039 (18)	0.17834 (18)	0.74106 (12)	0.0278 (3)	
H10	-0.0327	0.1440	0.7177	0.033*	
C11	0.1507 (2)	0.08271 (17)	0.75925 (12)	0.0292 (3)	
H11	0.1028	-0.0174	0.7484	0.035*	
C12	0.3002 (2)	0.13313 (17)	0.79310 (13)	0.0294 (3)	
H12	0.3548	0.0674	0.8064	0.035*	
C13	0.37211 (17)	0.27965 (16)	0.80794 (11)	0.0236 (3)	
H13	0.4753	0.3132	0.8306	0.028*	
C14	0.32522 (16)	0.67665 (15)	0.94660 (10)	0.0194 (3)	
C15	0.23729 (18)	0.57911 (17)	0.99534 (12)	0.0259 (3)	
H15	0.2122	0.4795	0.9727	0.031*	
C16	0.1859 (2)	0.6256 (2)	1.07644 (13)	0.0328 (4)	
H16	0.1258	0.5579	1.1086	0.039*	
C17	0.22211 (19)	0.7699 (2)	1.11016 (12)	0.0321 (4)	
H17	0.1880	0.8017	1.1661	0.038*	
C18	0.30798 (19)	0.86851 (18)	1.06277 (12)	0.0287 (3)	
H18	0.3324	0.9680	1.0859	0.034*	
C19	0.35860 (17)	0.82221 (16)	0.98128 (11)	0.0233 (3)	
H19	0.4168	0.8907	0.9487	0.028*	
C20	0.62870 (16)	0.68280 (16)	0.84325 (11)	0.0214 (3)	
C21	0.71474 (19)	0.6659 (2)	0.77435 (13)	0.0339 (4)	
H21	0.6690	0.6197	0.7092	0.041*	
C22	0.8665 (2)	0.7157 (3)	0.79983 (15)	0.0433 (5)	
H22	0.9237	0.7029	0.7521	0.052*	
C23	0.93509 (19)	0.7839 (2)	0.89410 (14)	0.0373 (4)	
H23	1.0390	0.8178	0.9112	0.045*	
C24	0.85144 (19)	0.80232 (19)	0.96333 (13)	0.0316 (4)	
H24	0.8978	0.8494	1.0282	0.038*	
C25	0.69961 (17)	0.75194 (17)	0.93803 (12)	0.0246 (3)	
H25	0.6430	0.7648	0.9861	0.029*	

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Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn	0.01785 (5)	0.01692 (5)	0.01786 (5)	0.00513 (4)	0.00269 (3)	0.00099 (3)
S1	0.02585 (18)	0.02457 (17)	0.01802 (16)	0.01231 (14)	0.00542 (13)	0.00314 (13)
S2	0.0303 (2)	0.02931 (19)	0.02422 (18)	0.01682 (16)	0.00519 (15)	0.00213 (14)
O1	0.0326 (6)	0.0268 (6)	0.0351 (6)	0.0064 (5)	0.0169 (5)	0.0082 (5)
C1	0.0189 (7)	0.0177 (6)	0.0196 (7)	0.0029 (5)	0.0037 (5)	0.0009 (5)
C2	0.0262 (7)	0.0245 (7)	0.0168 (7)	0.0056 (6)	0.0029 (5)	0.0002 (5)
C3	0.0256 (8)	0.0318 (8)	0.0222 (7)	0.0092 (6)	0.0080 (6)	0.0036 (6)
C4	0.0422 (11)	0.0335 (9)	0.0382 (10)	-0.0034 (8)	0.0184 (8)	0.0051 (8)
N1	0.0194 (6)	0.0211 (6)	0.0174 (6)	0.0059 (5)	0.0041 (4)	0.0027 (4)
C5	0.0347 (9)	0.0456 (10)	0.0231 (8)	0.0263 (8)	0.0067 (6)	0.0086 (7)
C6	0.0210 (9)	0.0262 (14)	0.0283 (10)	0.0093 (12)	0.0059 (7)	0.0029 (12)
O2	0.0243 (9)	0.0392 (9)	0.0445 (11)	0.0119 (8)	0.0048 (7)	-0.0067 (8)
C7	0.0675 (16)	0.0340 (11)	0.0552 (14)	0.0097 (10)	0.0002 (11)	0.0056 (10)
N1'	0.0194 (6)	0.0211 (6)	0.0174 (6)	0.0059 (5)	0.0041 (4)	0.0027 (4)
C5'	0.0347 (9)	0.0456 (10)	0.0231 (8)	0.0263 (8)	0.0067 (6)	0.0086 (7)
C6'	0.0210 (9)	0.0262 (14)	0.0283 (10)	0.0093 (12)	0.0059 (7)	0.0029 (12)
O2'	0.0243 (9)	0.0392 (9)	0.0445 (11)	0.0119 (8)	0.0048 (7)	-0.0067 (8)
C7'	0.0675 (16)	0.0340 (11)	0.0552 (14)	0.0097 (10)	0.0002 (11)	0.0056 (10)
C8	0.0220 (7)	0.0188 (6)	0.0155 (6)	0.0062 (5)	0.0038 (5)	0.0006 (5)
C9	0.0216 (7)	0.0254 (7)	0.0231 (7)	0.0065 (6)	0.0027 (5)	0.0006 (6)
C10	0.0235 (8)	0.0290 (8)	0.0254 (8)	0.0000 (6)	0.0058 (6)	-0.0021 (6)
C11	0.0390 (9)	0.0193 (7)	0.0273 (8)	0.0025 (6)	0.0133 (7)	-0.0003 (6)
C12	0.0383 (9)	0.0221 (7)	0.0330 (9)	0.0139 (7)	0.0127 (7)	0.0049 (6)
C13	0.0242 (7)	0.0239 (7)	0.0240 (7)	0.0094 (6)	0.0050 (6)	0.0026 (6)
C14	0.0196 (7)	0.0205 (6)	0.0177 (6)	0.0060 (5)	0.0028 (5)	0.0024 (5)
C15	0.0294 (8)	0.0217 (7)	0.0246 (7)	0.0037 (6)	0.0052 (6)	0.0050 (6)
C16	0.0325 (9)	0.0393 (9)	0.0264 (8)	0.0049 (7)	0.0126 (7)	0.0096 (7)
C17	0.0299 (9)	0.0455 (10)	0.0225 (8)	0.0127 (7)	0.0094 (6)	0.0002 (7)
C18	0.0330 (9)	0.0273 (8)	0.0258 (8)	0.0109 (7)	0.0056 (6)	-0.0037 (6)
C19	0.0247 (7)	0.0208 (7)	0.0231 (7)	0.0043 (6)	0.0064 (6)	0.0016 (5)
C20	0.0197 (7)	0.0213 (7)	0.0225 (7)	0.0054 (5)	0.0029 (5)	0.0040 (5)
C21	0.0242 (8)	0.0519 (11)	0.0231 (8)	0.0089 (7)	0.0044 (6)	-0.0002 (7)
C22	0.0242 (9)	0.0731 (15)	0.0324 (10)	0.0107 (9)	0.0105 (7)	0.0088 (9)
C23	0.0192 (8)	0.0489 (11)	0.0381 (10)	0.0011 (7)	0.0017 (7)	0.0124 (8)
C24	0.0270 (8)	0.0325 (8)	0.0289 (8)	0.0040 (7)	-0.0039 (6)	0.0029 (7)
C25	0.0257 (8)	0.0251 (7)	0.0223 (7)	0.0076 (6)	0.0029 (6)	0.0034 (6)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Sn—C8	2.1312 (14)	C6'—H6D	0.9900
Sn—C20	2.1357 (15)	O2'—C7'	1.530 (4)
Sn—C14	2.1608 (14)	C7'—H7D	0.9800
Sn—S1	2.4612 (4)	C7'—H7E	0.9800
Sn—S2	3.0992 (4)	C7'—H7F	0.9800
S1—C1	1.7629 (14)	C8—C13	1.3945 (19)

S2—C1	1.6781 (14)	C8—C9	1.397 (2)
O1—C3	1.415 (2)	C9—C10	1.386 (2)
O1—C4	1.421 (2)	C9—H9	0.9500
C1—N1'	1.3340 (19)	C10—C11	1.386 (2)
C1—N1	1.3340 (19)	C10—H10	0.9500
C2—N1'	1.4712 (18)	C11—C12	1.379 (3)
C2—N1	1.4712 (18)	C11—H11	0.9500
C2—C3	1.509 (2)	C12—C13	1.394 (2)
C2—H2A	0.9900	C12—H12	0.9500
C2—H2B	0.9900	C13—H13	0.9500
C3—H3A	0.9900	C14—C19	1.395 (2)
C3—H3B	0.9900	C14—C15	1.397 (2)
C4—H4A	0.9800	C15—C16	1.390 (2)
C4—H4B	0.9800	C15—H15	0.9500
C4—H4C	0.9800	C16—C17	1.379 (3)
N1—C5	1.4651 (19)	C16—H16	0.9500
C5—C6	1.409 (3)	C17—C18	1.381 (3)
C5—H5A	0.9900	C17—H17	0.9500
C5—H5B	0.9900	C18—C19	1.390 (2)
C6—O2	1.414 (3)	C18—H18	0.9500
C6—H6A	0.9900	C19—H19	0.9500
C6—H6B	0.9900	C20—C21	1.393 (2)
O2—C7	1.284 (3)	C20—C25	1.395 (2)
C7—H7A	0.9800	C21—C22	1.387 (3)
C7—H7B	0.9800	C21—H21	0.9500
C7—H7C	0.9800	C22—C23	1.382 (3)
N1'—C5'	1.4651 (19)	C22—H22	0.9500
C5'—C6'	1.692 (5)	C23—C24	1.382 (3)
C5'—H5C	0.9900	C23—H23	0.9500
C5'—H5D	0.9900	C24—C25	1.388 (2)
C6'—O2'	1.419 (4)	C24—H24	0.9500
C6'—H6C	0.9900	C25—H25	0.9500
C8—Sn—C20	119.54 (5)	O2'—C6'—C5'	110.1 (3)
C8—Sn—C14	104.97 (5)	O2'—C6'—H6C	109.6
C20—Sn—C14	107.25 (6)	C5'—C6'—H6C	109.6
C8—Sn—S1	110.54 (4)	O2'—C6'—H6D	109.6
C20—Sn—S1	118.49 (4)	C5'—C6'—H6D	109.6
C14—Sn—S1	90.94 (4)	H6C—C6'—H6D	108.2
C8—Sn—S2	84.48 (4)	C6'—O2'—C7'	121.0 (3)
C20—Sn—S2	87.42 (4)	O2'—C7'—H7D	109.5
C14—Sn—S2	154.45 (4)	O2'—C7'—H7E	109.5
S1—Sn—S2	63.534 (11)	H7D—C7'—H7E	109.5
C1—S1—Sn	97.95 (5)	O2'—C7'—H7F	109.5
C1—S2—Sn	78.60 (5)	H7D—C7'—H7F	109.5
C3—O1—C4	111.94 (14)	H7E—C7'—H7F	109.5
N1'—C1—S2	123.54 (11)	C13—C8—C9	118.59 (14)
N1—C1—S2	123.54 (11)	C13—C8—Sn	121.76 (11)

N1'—C1—S1	116.67 (10)	C9—C8—Sn	119.58 (10)
N1—C1—S1	116.67 (10)	C10—C9—C8	121.01 (14)
S2—C1—S1	119.79 (9)	C10—C9—H9	119.5
N1'—C2—C3	112.94 (12)	C8—C9—H9	119.5
N1—C2—C3	112.94 (12)	C11—C10—C9	119.81 (15)
N1—C2—H2A	109.0	C11—C10—H10	120.1
C3—C2—H2A	109.0	C9—C10—H10	120.1
N1—C2—H2B	109.0	C12—C11—C10	119.86 (15)
C3—C2—H2B	109.0	C12—C11—H11	120.1
H2A—C2—H2B	107.8	C10—C11—H11	120.1
O1—C3—C2	108.64 (13)	C11—C12—C13	120.63 (15)
O1—C3—H3A	110.0	C11—C12—H12	119.7
C2—C3—H3A	110.0	C13—C12—H12	119.7
O1—C3—H3B	110.0	C8—C13—C12	120.07 (15)
C2—C3—H3B	110.0	C8—C13—H13	120.0
H3A—C3—H3B	108.3	C12—C13—H13	120.0
O1—C4—H4A	109.5	C19—C14—C15	117.90 (13)
O1—C4—H4B	109.5	C19—C14—Sn	121.67 (11)
H4A—C4—H4B	109.5	C15—C14—Sn	120.33 (10)
O1—C4—H4C	109.5	C16—C15—C14	121.04 (15)
H4A—C4—H4C	109.5	C16—C15—H15	119.5
H4B—C4—H4C	109.5	C14—C15—H15	119.5
C1—N1—C5	122.66 (12)	C17—C16—C15	119.95 (16)
C1—N1—C2	120.73 (12)	C17—C16—H16	120.0
C5—N1—C2	116.61 (12)	C15—C16—H16	120.0
C6—C5—N1	122.02 (19)	C16—C17—C18	120.08 (15)
C6—C5—H5A	106.8	C16—C17—H17	120.0
N1—C5—H5A	106.8	C18—C17—H17	120.0
C6—C5—H5B	106.8	C17—C18—C19	120.01 (15)
N1—C5—H5B	106.8	C17—C18—H18	120.0
H5A—C5—H5B	106.7	C19—C18—H18	120.0
C5—C6—O2	107.8 (2)	C18—C19—C14	121.00 (15)
C5—C6—H6A	110.1	C18—C19—H19	119.5
O2—C6—H6A	110.1	C14—C19—H19	119.5
C5—C6—H6B	110.1	C21—C20—C25	118.04 (14)
O2—C6—H6B	110.1	C21—C20—Sn	124.74 (12)
H6A—C6—H6B	108.5	C25—C20—Sn	117.17 (11)
C7—O2—C6	109.2 (2)	C22—C21—C20	120.73 (16)
O2—C7—H7A	109.5	C22—C21—H21	119.6
O2—C7—H7B	109.5	C20—C21—H21	119.6
H7A—C7—H7B	109.5	C23—C22—C21	120.52 (17)
O2—C7—H7C	109.5	C23—C22—H22	119.7
H7A—C7—H7C	109.5	C21—C22—H22	119.7
H7B—C7—H7C	109.5	C22—C23—C24	119.56 (16)
C1—N1'—C5'	122.66 (12)	C22—C23—H23	120.2
C1—N1'—C2	120.73 (12)	C24—C23—H23	120.2
C5'—N1'—C2	116.61 (12)	C23—C24—C25	119.97 (16)
N1'—C5'—C6'	100.59 (18)	C23—C24—H24	120.0

N1'—C5'—H5C	111.7	C25—C24—H24	120.0
C6'—C5'—H5C	111.7	C24—C25—C20	121.18 (15)
N1'—C5'—H5D	111.7	C24—C25—H25	119.4
C6'—C5'—H5D	111.7	C20—C25—H25	119.4
H5C—C5'—H5D	109.4		
Sn—S2—C1—N1'	-176.86 (13)	N1'—C5'—C6'—O2'	160.9 (3)
Sn—S2—C1—N1	-176.86 (13)	C5'—C6'—O2'—C7'	82.6 (3)
Sn—S2—C1—S1	3.05 (7)	C13—C8—C9—C10	-1.3 (2)
Sn—S1—C1—N1'	176.12 (10)	Sn—C8—C9—C10	-178.46 (12)
Sn—S1—C1—N1	176.12 (10)	C8—C9—C10—C11	1.1 (2)
Sn—S1—C1—S2	-3.80 (9)	C9—C10—C11—C12	0.0 (2)
C4—O1—C3—C2	177.33 (13)	C10—C11—C12—C13	-0.9 (3)
N1'—C2—C3—O1	-66.76 (16)	C9—C8—C13—C12	0.4 (2)
N1—C2—C3—O1	-66.76 (16)	Sn—C8—C13—C12	177.47 (12)
S2—C1—N1—C5	-177.49 (12)	C11—C12—C13—C8	0.7 (2)
S1—C1—N1—C5	2.6 (2)	C19—C14—C15—C16	-0.6 (2)
S2—C1—N1—C2	2.9 (2)	Sn—C14—C15—C16	-177.05 (13)
S1—C1—N1—C2	-177.05 (10)	C14—C15—C16—C17	-0.3 (3)
C3—C2—N1—C1	-90.53 (17)	C15—C16—C17—C18	0.8 (3)
C3—C2—N1—C5	89.80 (17)	C16—C17—C18—C19	-0.3 (3)
C1—N1—C5—C6	-90.6 (2)	C17—C18—C19—C14	-0.6 (2)
C2—N1—C5—C6	89.0 (2)	C15—C14—C19—C18	1.1 (2)
N1—C5—C6—O2	178.09 (18)	Sn—C14—C19—C18	177.44 (12)
C5—C6—O2—C7	160.8 (2)	C25—C20—C21—C22	0.4 (3)
S2—C1—N1'—C5'	-177.49 (12)	Sn—C20—C21—C22	-176.82 (16)
S1—C1—N1'—C5'	2.6 (2)	C20—C21—C22—C23	-0.3 (3)
S2—C1—N1'—C2	2.9 (2)	C21—C22—C23—C24	0.0 (3)
S1—C1—N1'—C2	-177.05 (10)	C22—C23—C24—C25	0.3 (3)
C3—C2—N1'—C1	-90.53 (17)	C23—C24—C25—C20	-0.2 (3)
C3—C2—N1'—C5'	89.80 (17)	C21—C20—C25—C24	-0.1 (2)
C1—N1'—C5'—C6'	-85.0 (2)	Sn—C20—C25—C24	177.30 (13)
C2—N1'—C5'—C6'	94.66 (19)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg1 and Cg2 are the centroids of the C8—C13 and C14—C19 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C7—H7C $\cdots$ Cg1 <sup>i</sup>	0.98	2.94	3.821 (3)	151
C13—H13 $\cdots$ Cg2 <sup>ii</sup>	0.95	2.98	3.7979 (18)	145
C23—H23 $\cdots$ Cg2 <sup>iii</sup>	0.95	2.97	3.707 (2)	136

Symmetry codes: (i)  $-x, -y+1, -z+1$ ; (ii)  $-x+1, -y+1, -z+2$ ; (iii)  $x+1, y, z$ .