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# (*N*,*N*-Diallyldithiocarbamato-$\kappa^2 S,S'$)triphenyltin(IV) and bis(*N*,*N*-diallyldithiocarbamato-$\kappa^2 S,S'$)diphenyltin(IV): crystal structure, Hirshfeld surface analysis and computational study

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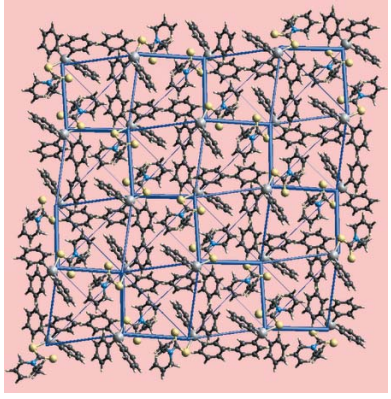
The crystal and molecular structures of the title organotin dithiocarbamate compounds, $[Sn(C_6H_5)_3(C_7H_{10}NS_2)]$ (I) and $[Sn(C_6H_5)_2(C_7H_{10}NS_2)_2]$ (II), present very distinct tin atom coordination geometries. In (I), the dithiocarbamate ligand is asymmetrically coordinating with the resulting $C_3S_2$ donor set defining a coordination geometry intermediate between square-pyramidal and trigonal–bipyramidal. In (II), two independent molecules comprise the asymmetric unit, which differ in the conformations of the allyl substituents and in the relative orientations of the tin-bound phenyl rings. The dithiocarbamate ligands in (II) coordinate in an asymmetric mode but the Sn—S bonds are more symmetric than observed in (I). The resulting $C_2S_4$ donor set approximates an octahedral coordination geometry with a *cis*-disposition of the *ipso*-carbon atoms and with the more tightly bound sulfur atoms approximately *trans*. The only directional intermolecular contacts in the crystals of (I) and (II) are of the type phenyl-C—H$\cdots\pi$(phenyl) and vinylidene-C—H$\cdots\pi$(phenyl), respectively, with each leading to a supramolecular chain propagating along the *a*-axis direction. The calculated Hirshfeld surfaces emphasize the importance of H$\cdots$H contacts in the crystal of (I), *i.e.* contributing 62.2% to the overall surface. The only other two significant contacts also involve hydrogen, *i.e.* C$\cdots$H/H$\cdots$C (28.4%) and S$\cdots$H/H$\cdots$S (8.6%). Similar observations pertain to the individual molecules of (II), which are clearly distinguishable in their surface contacts, with H$\cdots$H being clearly dominant (59.9 and 64.9%, respectively) along with C$\cdots$H/H$\cdots$C (24.3 and 20.1%) and S$\cdots$H/H$\cdots$S (14.4 and 13.6%) contacts. The calculations of energies of interaction suggest dispersive forces make a significant contribution to the stabilization of the crystals. The exception is for the C—H$\cdots\pi$ contacts in (II) where, in addition to the dispersive contribution, significant contributions are made by the electrostatic forces.

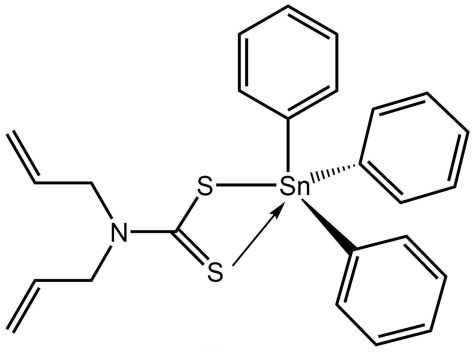




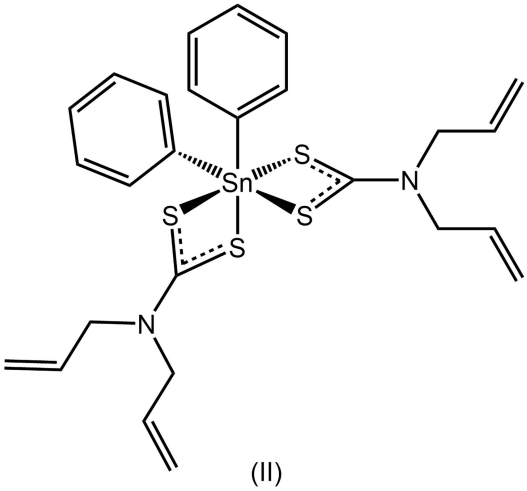
## 1. Chemical context

Dithiocarbamate anions of general formula $^-S_2CNRR'$, $R/R'$ = H, alkyl and aryl, are readily prepared from the facile reaction of an amine with $CS_2$ in the presence of base. Thus, the number of derivatives which can be prepared is largely dictated by the availability of amines and hence, an enormous range of dithiocarbamate anions are available for complexation to metals/heavy elements. A key interest in developing metal/heavy element compounds of dithiocarbamates relates to their biological potential (Hogarth, 2012). In the context of

anti-cancer properties, a number of recent reports have described the efficacy of phosphanegold (Jamaludin *et al.*, 2013), zinc (Tan *et al.*, 2015) and bismuth (Ishak *et al.*, 2014) dithiocarbamates, buoyed by the observation that many of these species promote cancer cell death by apoptosis; bismuth derivatives exhibit *in vivo* anti-tumour activity (Li *et al.*, 2007). Organotin compounds are well known for their anti-cancer potential (Gielen & Tiekink, 2005) and there is a strong body of literature on organotin dithiocarbamates in this context (Tiekink, 2008).




(I)




(II)

In the past few years, there has been a resurgence of interest in the anti-cancer activity of organotin dithiocarbamates (Khan *et al.*, 2015; Mohamad, Awang, Kamaludin *et al.*, 2016) and very recently, a report on the *in vitro* cytotoxicity trial of several tin diallyldithiocarbamate compounds was described as well as a preliminary assessment of anti-microbial activity (Adeyemi *et al.*, 2019); some phosphane-gold(I) and phosphane-silver(I) dithiocarbamates are known to be bactericidal based on pharmacokinetic studies (Sim *et al.*, 2014; Tan, Tan *et al.*, 2019). The aforementioned report on tin diallyldithiocarbamate compounds (Adeyemi *et al.*, 2019) also presented the first crystal-structure determinations for tin compounds of diallyldithiocarbamate. In a continuation of recent structural studies in this area (Mohamad *et al.*, 2017, 2018*a*,*b*; Haezam *et al.*, 2019), herein, two organotin compounds of diallyldithiocarbamate, $(C_6H_5)_3Sn[S_2CN(CH_2C(H)=CH_2)_2]$, (I), and $(C_6H_5)_2Sn[S_2CN(CH_2C(H)=CH_2)_2]_2$, (II), have been synthesized and studied by X-ray crystallography. In addition, the supramolecular associations in their crystals have been evaluated by Hirshfeld surface analyses and computational chemistry.

**Table 1**
Selected geometric parameters (Å, °) for (I).

| Parameter | (I) | Parameter | (I) |
|---|---|---|---|
| Sn—S1 | 2.4749 (4) | Sn—S2 | 2.9456 (5) |
| Sn—C11 | 2.1427 (19) | Sn—C21 | 2.130 (2) |
| Sn—C31 | 2.1673 (19) | C1—S1 | 1.7559 (19) |
| C1—S2 | 1.6894 (19) | C1—N1 | 1.330 (3) |
| S1—Sn—S2 | 65.470 (14) | C11—Sn—C21 | 111.15 (7) |
| C11—Sn—C31 | 104.14 (7) | C21—Sn—C31 | 107.13 (7) |
| S1—Sn—C11 | 128.76 (5) | S2—Sn—C31 | 156.01 (5) |

## 2. Structural commentary

The tin atom in (I), Fig. 1, is coordinated by three *ipso*-carbon atoms of the phenyl groups as well as by an asymmetrically bound dithiocarbamate anion, Table 1. There is a relatively large disparity in the Sn—S separations, *i.e.* $\Delta$(Sn—S) = [(Sn—$S_{long}$) - (Sn—$S_{short}$)] = 0.47 Å, indicating that the Sn—S2 interaction is weak. Evidence in support of this conclusion is seen in the pattern of C—S bond lengths. Thus, the C1—S2 bond involving the less tightly bound S2 atom is about 0.07 Å shorter than the analogous bond with the tightly bound S1 atom. Nevertheless, there is a clear influence exerted by the S2 atom upon the Sn—C bond lengths with the Sn—C31 bond being appreciably longer than the other Sn—C bonds. This is traced to the *trans* effect exerted by the S2 atom as this forms a S2—Sn—C31 angle 156.01 (5)°. It is noted that there is no other (approximate) *trans* angle subtended at the tin atom in (I). Assuming a five-coordinate, $C_3S_2$, geometry, the range of

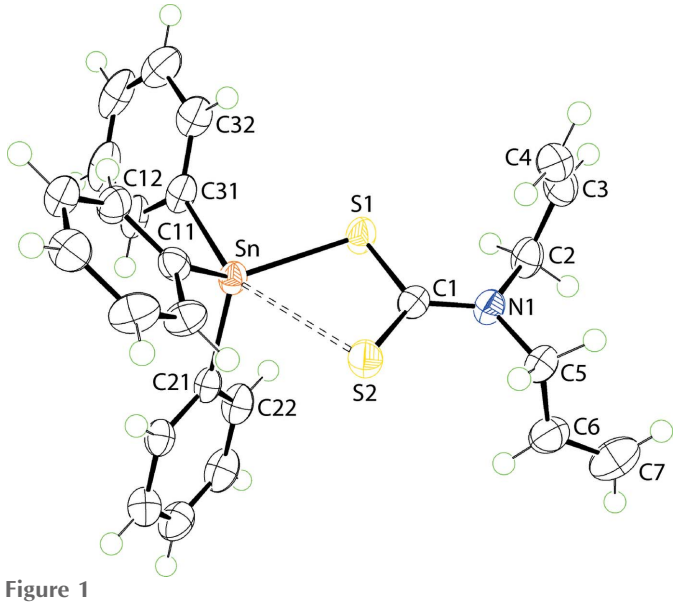



**Figure 1**
The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

angles subtended at the tin atom is 65.470 (14)°, for the S1—Sn—S2 chelate angle, to the aforementioned *trans* angle. The value of $\tau$ is a convenient descriptor for the assignment of a five-coordinate geometry, which ranges in value from 0.0 for an ideal square pyramid to 1.0 for an ideal trigonal bipyramid (Addison *et al.*, 1984). The value of $\tau$ the case of (I) is 0.45, which is indicative of an intermediate geometry with a slight tendency towards square pyramidal. On the other hand, should the coordination geometry be considered $C_3S$ tetrahedral, *i.e.* the weak Sn—S2 bond was ignored, the range of tetrahedral angles would be 91.01 (5)°, for S1—Sn—C31, to 128.76 (5)°, for S1—Sn—C11. Finally, it is noted the C1—N1 bond length of 1.330 (3) Å is consistent with significant double-bond character in this bond, which arises from a major contribution of the $^{2-}S_2C{=}N^+(CH_2C(H){=}CH_2)_2$ canonical form to the electronic structure of the dithiocarbamate ligand.

A distinct coordination geometry for the tin atoms is noted for (II), Fig. 2, for which two independent molecules comprise the crystallographic asymmetric unit. The tin atom in each molecule is coordinated by two *ipso*-carbon atoms of the phenyl groups as well as by two asymmetrically bound dithiocarbamate anions, Table 2. There is a disparity in the Sn—S separations, *i.e.* Δ(Sn—S) = 0.19 and 0.11 Å, for the S1- and S3-dithiocarbamate anions of the first independent molecule; the comparable values for the second molecule are similar at 0.21 and 0.11 Å. The disparities in Δ(Sn—S) are reflected in the associated C—S bond distances, Table 2. Gratifyingly, the greater differences in C—S bonds, *i.e.* 0.03 and 0.04 Å for the S1-dithiocarbamate anions of each independent molecule, are correlated with the greater values in Δ(Sn—S). The C1—N1 and C8—N2 bond lengths in both molecules are short for the reasons mentioned for (I) above. The $C_2S_4$ coordination geometry is based on an octahedron and has a *cis*-disposition of the *ipso*-carbon atoms with the more tightly bound sulfur atoms close to being *trans*. A partial explanation of the lengthening of the Sn—S2 and Sn—S4 bonds relates to the *trans*-influence exerted by the phenyl substituents approximately opposite the S2 and S4 atoms.

A view of the superimposition of the two molecules comprising the asymmetric unit in (II) is shown in Fig. 3 whereby the Sn1- and inverted-Sn2-molecules are overlapped so that two chelate rings, *i.e.* (Sn1,S1,S2,C1) and (Sn2,S3,S4,C8), are coincident. This shows there are non-trivial conformational differences between the molecules. While the dihedral angles between the two phenyl substituents are equal within experimental error in the two molecules, *i.e.* 81.28 (13) and 81.63 (14)°, more telling are the angles they form with the respective, *cis*-disposed chelate rings, *i.e.* 81.06 (10) and 35.93 (10)° for the Sn1-molecule and 15.35 (11) and 74.71 (6)° for the Sn2-molecule. Differences are also noted in the relative orientations of the allyl substituents. Thus, for the overlapped dithiocarbamate ligands, the N1—

**Table 2**
Selected geometric parameters (Å, °) for the two independent molecules in (II).

| Parameter | Sn1-molecule | Sn2-molecule |
|---|---|---|
| Sn—S1 | 2.5501 (6) | 2.5585 (7) |
| Sn—S2 | 2.7393 (7) | 2.7664 (7) |
| Sn—S3 | 2.5726 (7) | 2.5700 (6) |
| Sn—S4 | 2.6754 (6) | 2.6750 (6) |
| C1—S1 | 1.742 (3) | 1.740 (3) |
| C1—S2 | 1.710 (3) | 1.704 (3) |
| C8—S3 | 1.738 (3) | 1.733 (3) |
| C8—S4 | 1.715 (3) | 1.716 (3) |
| C1—N1 | 1.326 (3) | 1.328 (4) |
| C8—N2 | 1.318 (3) | 1.327 (3) |
| | | |
| S1—Sn—S2 | 67.824 (19) | 67.18 (2) |
| S3—Sn—S4 | 67.97 (2) | 68.69 (2) |
| S1—Sn—S3 | 154.38 (2) | 149.00 (2) |
| S2—Sn—C21 | 159.42 (7) | 161.40 (7) |
| S4—Sn—C15 | 160.59 (7) | 159.91 (7) |
| C15—Sn—C21 | 99.84 (9) | 103.34 (9) |
| | | |
| N1—C2—C3—C4 | 12.5 (4) | 9.9 (4)[a] |
| N1—C5—C6—C7 | −122.3 (3) | 13.3 (4)[a] |
| N2—C9—C10—C11 | 105.3 (3) | 105.2 (3)[a] |
| N2—C12—C13—C14 | 110.9 (4) | 114.6 (4)[a] |

Note: (*a*) for ease of comparison, the torsion angles are for the inverted Sn2-molecule.

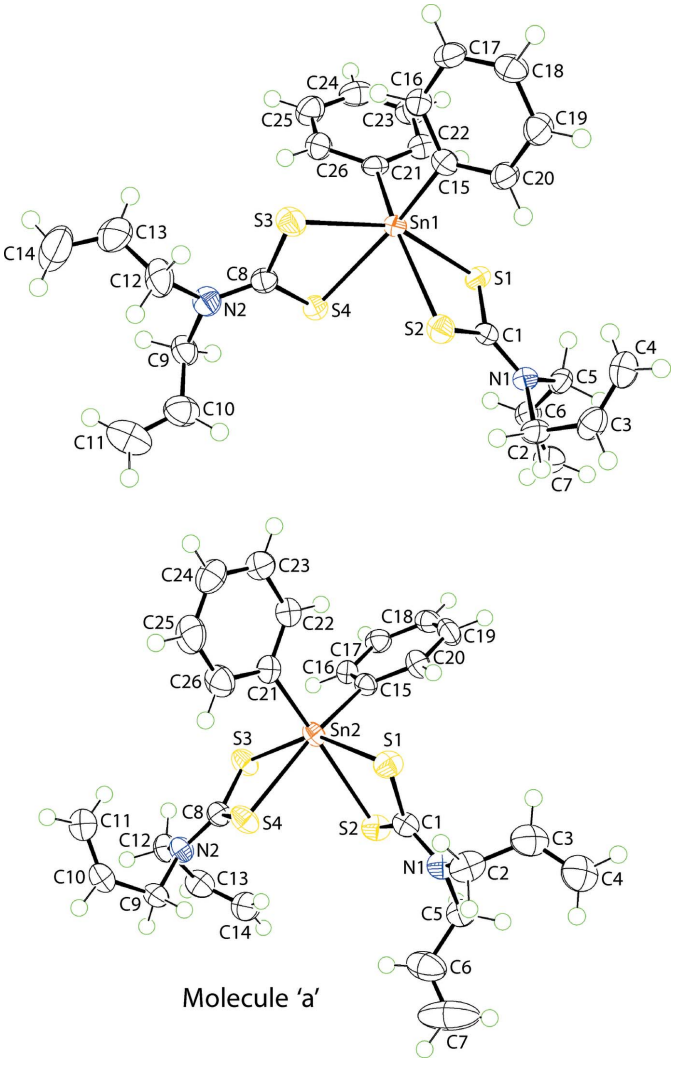



**Figure 2**
The molecular structures of the two independent molecules comprising the asymmetric unit of (II) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

**Table 3**
Hydrogen-bond geometry (Å, °) for (I).

*Cg*1 and *Cg*2 are the centroids of the (C21–C26) and (C31–C36) rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13···*Cg*1$^{i}$ | 0.95 | 2.92 | 3.605 (2) | 130 |
| C23—H23···*Cg*2$^{ii}$ | 0.95 | 2.99 | 3.720 (3) | 134 |

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

**Table 4**
Hydrogen-bond geometry (Å, °) for (II).

*Cg*1 and *Cg*2 are the centroids of the (C15*A*–C20*A*) and (C21*A*–C26*A*) rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7*A*···*Cg*1$^{i}$ | 0.95 | 2.83 | 3.774 (3) | 172 |
| C7—H7*B*···*Cg*2$^{ii}$ | 0.95 | 2.92 | 3.582 (3) | 128 |

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

C5—C6—C7 torsion angle of −122.3 (3)° is an outlier with respect to the other torsion angles with the direct equivalent angle for the inverted Sn2-molecule being 13.3 (4)°. While the N—C—C—C torsion angles for the second pair of dithiocarbamate ligands are similar, Table 2, there is a misalignment of these ligands as seen in the dihedral angle formed between the chelate rings of 80.98 (5) and 76.55 (6)° for the Sn1- and Sn2-molecules, respectively.

The difference in coordination modes of the dithiocarbamate ligands and coordination geometries are related, at least in part, to the different Lewis acid strength of the tin atoms, with the Lewis acidity in the triphenyltin species being significantly less than that in the diphenyltin species.

## 3. Supramolecular features

The only directional point of contact between molecules based on the distance criteria in *PLATON* (Spek, 2020) are phenyl-C—H···$\pi$(phenyl) interactions, Table 3. Here, the (C21–C26) ring is pivotal by donating a C—H atom to a symmetry-related (C31–C36) ring and the same time accepting a phenyl-C—H···$\pi$(phenyl) interaction from a (C11–C16) ring to construct a linear, supramolecular chain aligned along the *a*-axis direction, Fig. 4(*a*). The chains assemble in the crystal without directional interactions between them, Fig. 4(*b*).

The molecular packing in (II) is also largely devoid of directional interactions. Indeed, the only connections evident are vinylidene-C—H···$\pi$(phenyl) interactions, Table 4, which serve to link the independent molecules comprising the asymmetric unit into a supramolecular chain aligned along the *a*-axis direction. In essence, the vinylidene-hydrogen atoms of the Sn1-molecule bridge translationally related Sn2-molecules into a linear chain, Fig. 5(*a*). The chains pack without directional interactions between them, Fig. 5(*b*).

## 4. Hirshfeld surface analysis

In order to gain further insight into the molecular packing of each of (I) and (II), Hirshfeld surface calculations were

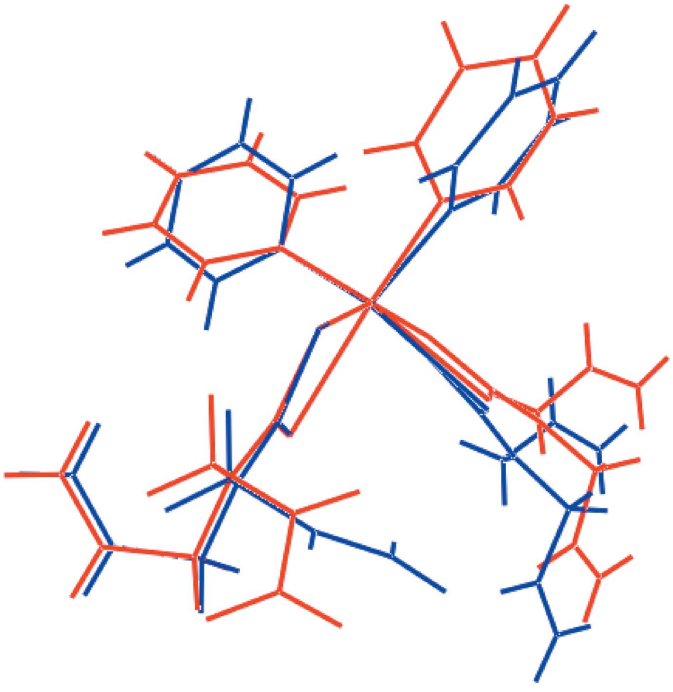


**Figure 3**
Overlay diagram of the independent molecules comprising the asymmetric unit of (II): (*a*) Sn1-containing molecule (red image) and (*b*) inverted-Sn2-molecule (blue). The molecules are overlapped so that the (Sn1,S1,S2,C1) and (Sn2,S3,S4,C8) residues are coincident.

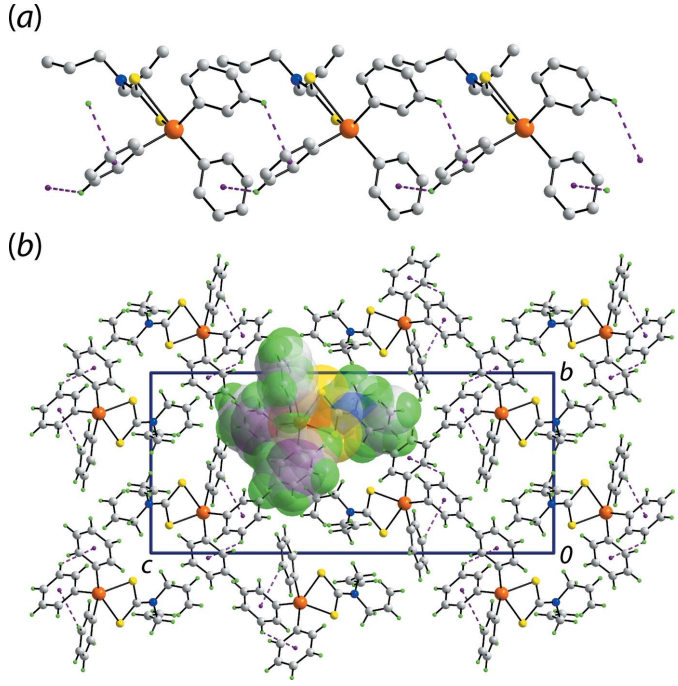



**Figure 4**
Molecular packing in the crystal of (I): (*a*) supramolecular chain along the *a*-axis direction sustained by phenyl-C—H···$\pi$(phenyl) interactions shown as purple dashed lines (non-participating hydrogen atoms have been removed) and (*b*) a view of the unit-cell contents in projection down the *a* axis with one chain highlighted in space-filling mode.

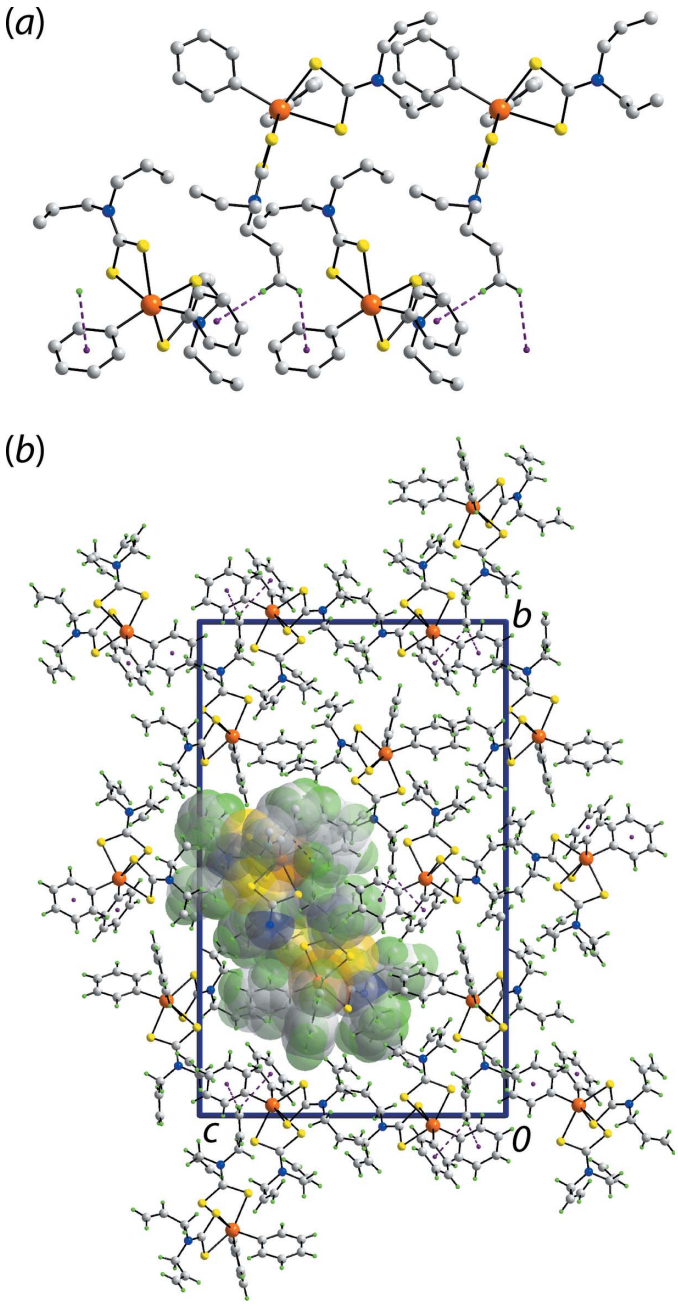



**Figure 5**
Molecular packing in the crystal of (II): (*a*) supramolecular chain along the *a*-axis direction sustained by methylene-C—H···$\pi$(phenyl) interactions shown as purple dashed lines (non-participating hydrogen atoms have been removed) and (*b*) a view of the unit-cell contents in projection down the *a* axis with one chain highlighted in space-filling mode.

performed with *Crystal Explorer 17* (Turner *et al.*, 2017) following literature protocols (Tan, Jotani *et al.*, 2019). The calculations highlight the influence of the discussed C—H···$\pi$ interactions (Tables 3 and 4) as well the short interatomic contacts collated in Table 5. The short interatomic contacts are indicated as diminutive or faint-red spots near the participating atoms on the Hirshfeld surfaces mapped over $d_{norm}$ for (I) and (II) in Figs. 6 and 7, respectively. Further, the donors and acceptors of the intermolecular C—H···$\pi$ contacts for

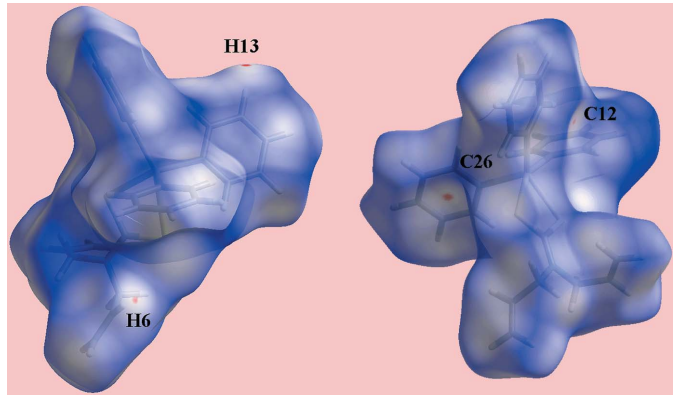



**Figure 6**
Two views of Hirshfeld surface for (I) mapped over $d_{norm}$ in the range −0.028 to +1.257 arbitrary units.

both (I) and (II) are evident as the blue bumps and red concave regions, respectively, on the Hirshfeld surfaces mapped with shape-index property shown in Fig. 8. In the absence of potential hydrogen bonds in (I) and (II), both the blue and red regions corresponding to positive and negative electrostatic potential, respectively, on Hirshfeld surfaces mapped over electrostatic potential in Fig. 9 and arise owing to the polarization of charges towards the participating residues.

The overall two-dimensional fingerprint plots for (I) and the individual molecules of (II) are illustrated in Fig. 10(*a*), and those delineated into H···H, C···H/H···C and S···H/H···S contacts are illustrated in Fig. 10(*b*)–(*d*), respectively. The percentage contributions from different atom–atom contacts to the Hirshfeld surfaces of (I), Sn1- and Sn2-molecules of (II) are quantitatively summarized in Table 6. In the fingerprint

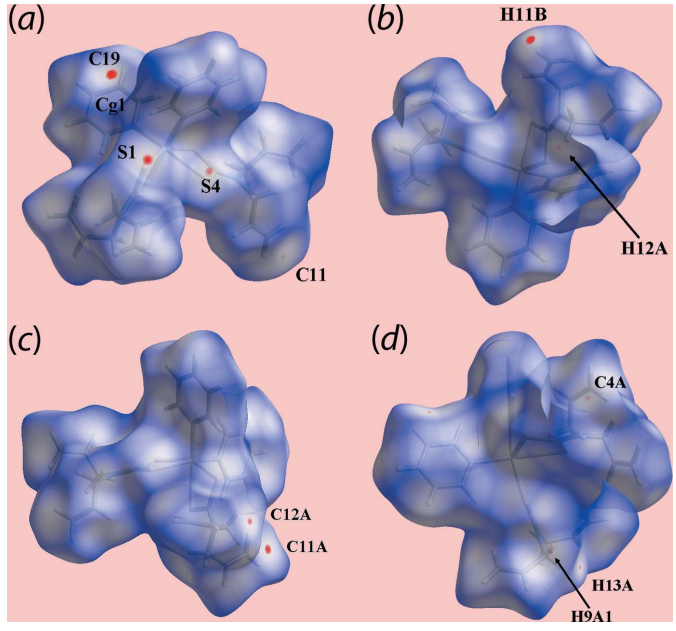



**Figure 7**
Views of the Hirshfeld surfaces for (II) mapped over $d_{norm}$ for the (*a*) and (*b*) Sn1-molecule in the range −0.026 to +1.372 arbitrary units, and (*c*) and (*d*) Sn2-molecule in the range −0.027 to +1.383 arbitrary units.

**Table 5**
Summary of short interatomic contacts (Å) in (I) and (II)[a].

| Contact | Distance | Symmetry operation |
|---|---|---|
| (I) | | |
| C12···H6 | 2.76 | $-1+x, y, z$ |
| C16···H5*B* | 2.80 | $1-x, -y, 1-z$ |
| C25···H4*B* | 2.78 | $x, \frac{1}{2}-y, -\frac{1}{2}+z$ |
| C26···H13 | 2.74 | $1+x, y, z$ |
| C33···H2*B* | 2.79 | $1-x, 1-y, 1-z$ |
| H15···H24 | 2.19 | $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| S1···H7*B* | 2.91 | $-1+x, y, z$ |
| S1···H2*A* | 2.96 | $1-x, 1-y, 1-z$ |
| (II) | | |
| S1···C11*A* | 3.455 (3) | $1-x, 1-y, 1-z$ |
| S4···C12*A* | 3.473 (3) | $1-x, 1-y, 1-z$ |
| C11···C23*A* | 3.386 (5) | $x, y, z$ |
| C11···H23*A* | 2.81 | $x, y, z$ |
| C19···H11*B* | 2.71 | $1+x, \frac{1}{2}-y, \frac{1}{2}+z$ |
| C21···H12*D* | 2.78 | $1-x, 1-y, 1-z$ |
| H12*A*···H9*A*2 | 2.16 | $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$ |
| H17···H26 | 2.18 | $1+x, y, z$ |
| C4*A*···H9*A*1 | 2.75 | $1-x, 1-y, -z$ |
| S1*A*···H18 | 2.91 | $1-x, \frac{1}{2}-y, -\frac{1}{2}+z$ |
| H17···H13*A* | 2.33 | $2-x, 1-y, 1-z$ |

Note: (*a*) The interatomic distances are calculated in *Crystal Explorer 17* (Turner *et al.*, 2017) whereby the *X*—H bond lengths are adjusted to their neutron values.

plot delineated into H···H contacts for (I), Fig. 10(*b*), a pair of small and proximate peaks at $d_e + d_i$ ~2.2 Å results from the presence of a short interatomic contact between the phenyl-H15 and H24 atoms, Table 5. The presence of a single peak at $d_e + d_i$ ~2.2 Å in the analogous plot for the Sn1-molecule of (II) is due to the short H···H contact between the phenyl-H17 and H26 atoms. Another short interatomic H···H contact

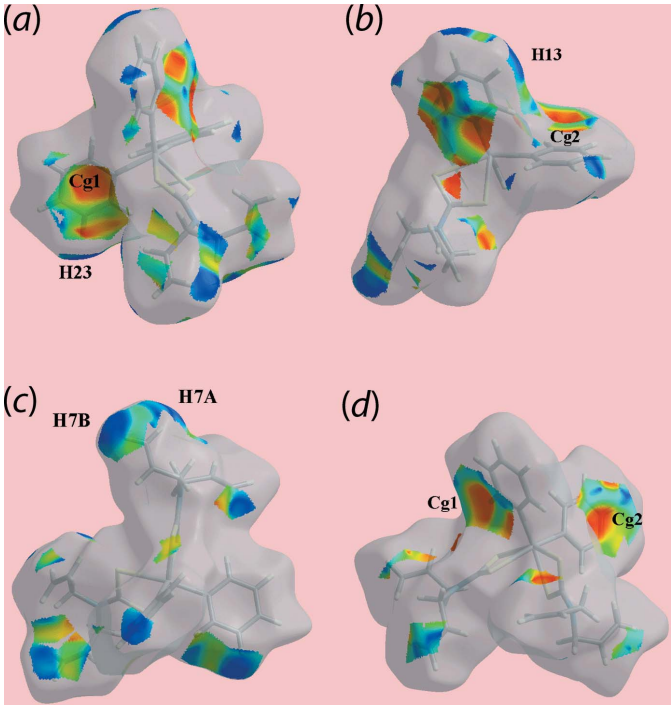



**Figure 8**
Views of Hirshfeld surfaces mapped with the shape-index property highlighting donors and acceptors of the intermolecular C—H···$\pi$ contacts for (*a*) and (*b*) (I), and (*c*) and (*d*) (II).

**Table 6**
Percentage contributions of interatomic contacts to the Hirshfeld surface for (I), the Sn1-molecule in (II) and the Sn2-molecule in (II).

| Contact | Percentage contribution | | |
|---|---|---|---|
| | (I) | Sn1-molecule in (II) | Sn2-molecule in (II) |
| H···H | 62.2 | 59.9 | 64.9 |
| C···H/H···C | 28.4 | 24.3 | 20.1 |
| S···H/H···S | 8.6 | 14.4 | 13.6 |
| N···H/H···N | 0.1 | 0.8 | 0.7 |
| C···C | 0.4 | 0.3 | 0.1 |
| S···C/C···S | 0.2 | 0.4 | 0.6 |
| Sn···H/H···Sn | 0.1 | 0.0 | 0.0 |

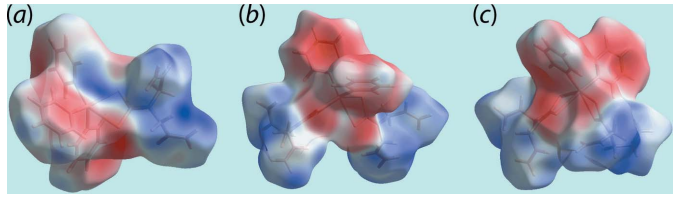



**Figure 9**
Views of Hirshfeld surfaces mapped over the electrostatic potential (the red and blue regions represent negative and positive electrostatic potentials, respectively) for (*a*) (I) in the range −0.032 to +0.043 atomic units (a.u.), (*b*) the Sn1-molecule in (II) in the range −0.039 to +0.040 a.u. and (*c*) the Sn2-molecule in (II) in the range −0.038 to +0.047 a.u.

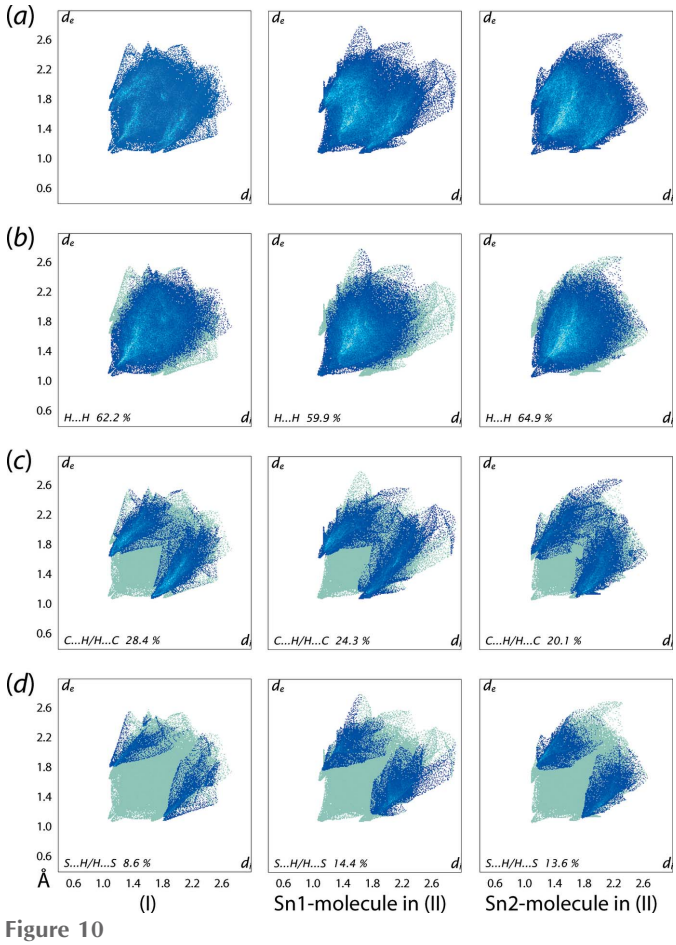



**Figure 10**
(*a*) A comparison of the full two-dimensional fingerprint plot for (I) and for the Sn1- and Sn2-molecules of (II), and those delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) S···H/H···S contacts.

**Table 7**
Summary of interaction energies (kJ mol$^{-1}$) calculated for (I) and (II).

| Contact | $R$ (Å) | $E_{ele}$ | $E_{pol}$ | $E_{dis}$ | $E_{rep}$ | $E_{tot}$ |
|---|---|---|---|---|---|---|
| (I)[a] | | | | | | |
| H13···C26$^{i}$ + C13—H13···*Cg*(C21–C26)$^{i}$ + C23—H23···*Cg*(C31–C36)$^{i}$ + H6···C12$^{i}$ + H7*B*···S1$^{i}$ | 8.06 | −13.8 | −5.6 | −68.5 | 42.5 | −45.0 |
| C16···H5*B*$^{ii}$ | 8.42 | −21.8 | −5.6 | −52.2 | 29.1 | −49.3 |
| C33···H2*B*$^{iii}$ + S1···H2*A*$^{iii}$ | 8.00 | −21.2 | −7.0 | −59.2 | 29.5 | −55.6 |
| C25···H4*B*$^{iv}$ | 9.91 | −0.6 | −0.8 | −23.3 | 8.4 | −15.2 |
| H15···H24$^{v}$ | 12.94 | −2.6 | −0.5 | −12.5 | 9.1 | −6.9 |
| (II)[b] | | | | | | |
| S1···C11*A*$^{i}$ + S4···C12*A*$^{i}$ + C7—H7*B*···*Cg*(C21*A*–C26*A*)$^{i}$ + C21···H12*D*$^{i}$ | 8.68 | −25.4 | −8.6 | −67.8 | 44.0 | −57.0 |
| C4*A*···H9*A*1$^{ii}$ | 9.0 | −28.8 | −7.3 | −69.0 | 49.0 | −56.5 |
| C7—H7*A*···*Cg*(C15*A*–C20*A*)$^{iii}$ + H17···H13*A*$^{iii}$ | 9.21 | −19.6 | −7.4 | −61.3 | 33.7 | −52.6 |
| H17···H26$^{iv}$ | 9.62 | −12.0 | −5.0 | −51.2 | 25.9 | −40.6 |
| C11···C23*A*$^{v}$ | 9.93 | −10.2 | −2.9 | −44.1 | 23.5 | −33.0 |
| C11···H23*A*$^{v}$ | | | | | | |
| H12*A*···H9*A*2$^{vi}$ | 10.81 | −5.9 | −2.4 | −30.6 | 14.5 | −23.4 |
| S1*A*···H18$^{vii}$ | 10.11 | −5.2 | −3.6 | −34.3 | 18.9 | −23. |
| C19···H11*B*$^{viii}$ | 12.51 | −7.4 | −2.6 | −20.5 | 9.8 | −19.8 |

Notes: (*a*) Symmetry operations for (I): (i) $-1+x, y, z$; (ii) $1-x, -y, 1-z$; (iii) $1-x, 1-y, 1-z$; (iv) $x\,\frac{1}{2}-y, -\frac{1}{2}+z$; (v) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$. (*b*) Symmetry operations for (II): (i) $1-x, 1-y, 1-z$; (ii) $1-x, 1-y, -z$; (iii) $2-x, 1-y, 1-z$; (iv) $1+x, y, z$; (v) $x, y, z$; (vi) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (vii) $1-x, \frac{1}{2}-y, -\frac{1}{2}+z$; (viii) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$.

involving the H17 and H18*A* atoms of the Sn1-molecule and the H9*A*2 and H13*A* atoms of the Sn2-molecule, Table 5, are evident as the pair of peaks at $d_e + d_i$ ~2.2 Å and at $d_e + d_i$ ~2.3 Å in the corresponding delineated plot for the Sn2-molecule.

The presence of short interatomic C···H/H···C contacts in each of (I) and (II), summarized in Table 5, are evident as the forceps-like tips at $d_e + d_i$ ~2.8 Å in Fig. 10(*a*). Also, the intermolecular C—H···$\pi$ contacts are characterized as a pair of wings in their respective delineated plots shown in Fig. 10(*c*). The short interatomic C···H/H···C contacts in the crystal of (II) appear as a pair of forceps-like tips at $d_e + d_i$ ~2.7 Å for the Sn1-molecule and as two pairs of similar adjoining tips at the same distances $d_e + d_i$ ~2.8 Å for the Sn2-molecule in the plots of Fig. 10(*c*). For (I), in the fingerprint plot delineated into S···H/H···S contacts of Fig. 10(*d*), the short interatomic contacts involving thiocarbamate-S1 and the H2*A* and H7*B* atoms are evident as the pair of conical tips at $d_e + d_i$ ~2.9 Å. Similar contacts in the crystal of (II) are also evident as the conical tips at $d_e + d_i$ ~2.9 Å in Fig. 10(*d*) in the upper and lower regions of the plots for the Sn1- and Sn2-molecules, respectively.

## 5. Computational chemistry

The pairwise interaction energies between the molecules within the crystals of (I) and (II) were calculated by summing up four energy components, namely the electrostatic ($E_{ele}$), polarization ($E_{pol}$), dispersion ($E_{dis}$) and exchange-repulsion ($E_{rep}$) energies, in accord with literature protocols (Turner *et al.*, 2017). In the present analysis, these energies were obtained by using the wave function calculated at the HF/3-21G level of theory. The specific contacts and associated energies are quantitatively summarized in Table 7. An analysis of these energies for (I) and (II) reveals that the dispersive component makes the major contribution to all the specified intermolecular interactions in the crystals of (I) and (II). However, as clearly evident from the relevant interaction energies listed in Table 7 and in the Hirshfeld surfaces mapped over the electrostatic potential of Fig. 9, where intense blue and red regions are apparent around the donors and acceptors, the C—H···$\pi$ contacts in (II) have more significant contributions from the $E_{ele}$ component, in contrast to mainly dispersive contributions in the case of (I).

A further noticeable observation about the strength of the intermolecular interactions from Table 7 is that those intermolecular contacts arising from the same pair of symmetry-related molecules have the greater interaction energies. The magnitudes of intermolecular energies were also represented graphically by energy frameworks to view the supramolecular architecture of both the crystals through cylinders joining the centroids of molecular pairs using red, green and blue colour codes for the $E_{ele}$, $E_{disp}$ and $E_{tot}$ terms, respectively. In summary, the images of Fig. 11 highlight the importance of dispersion forces in the crystals of (I) and (II).

## 6. Database survey

As a result of having several important applications, such as biological activity as alluded to in the *Chemical Context*, a

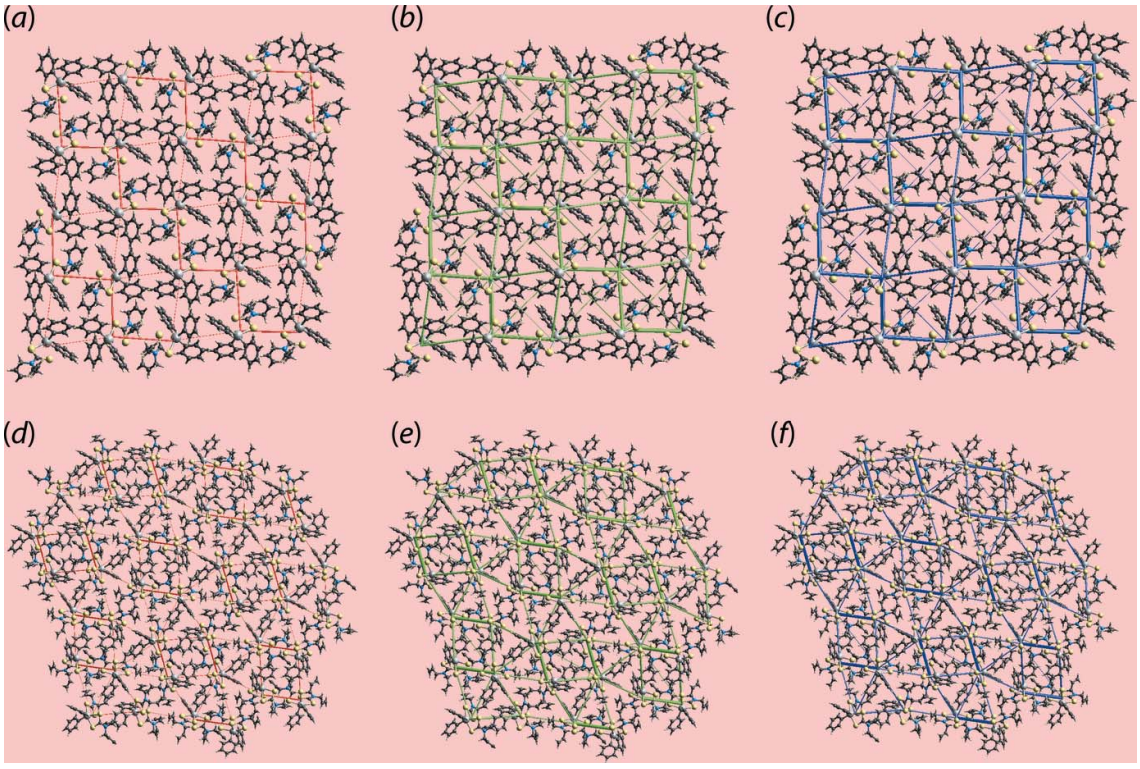



**Figure 11**
The energy frameworks calculated for (I) viewed down the *a*-axis direction showing the (*a*) electrostatic potential force, (*b*) dispersion force and (*c*) total energy. The corresponding plots for (II), viewed down the *a*-axis direction are shown in (*d*)–(*f*), respectively. The energy frameworks were adjusted to the same scale factor of 50 with a cut-off value of 5 kJ mol$^{-1}$ within 2 × 2 × 2 unit cells.

relatively large number of organotin dithiocarbamates have been synthesized and investigated by X-ray crystallography (Tiekink, 2008). The coordination geometry described for (I) conforms with literature expectations in that all $R_3Sn(S_2CNR'R'')$ molecules conform to this structural motif (Tiekink, 2008; Mohamad *et al.*, 2018*a*). The Sn—S1 bond length in (I) of 2.4749 (4) Å is slightly longer that the average Sn—$S_{short}$ bond of 2.47 Å in all $Ph_3Sn(S_2CNR'R'')$ structures, while the Sn—S2 bond of 2.9456 (5) Å in (I) is about 0.10 Å shorter than the average Sn—$S_{long}$ of 3.04 Å in these structures. Consistent with these trends, Δ(Sn—S) in (I) of 0.47 Å is less than the average Δ(Sn—S) value of 0.57 Å calculated from all $Ph_3Sn(S_2CNR'R'')$ structures.

Greater structural diversity is noted for $R_2Sn(S_2CNR'R'')_2$ (Tiekink, 2008), including differences in coordination numbers and geometries (Mohamad, Awang, Jotani *et al.*, 2016). Of the now, 17 structures of the general formula $Ph_2Sn(S_2CNR'R'')_2$, nine adopt the *cis*-$C_2S_4$ structural motif exemplified by (II), including the two polymorphs of $Ph_2Sn(S_2CNEt_2)_2$ (Lindley & Carr, 1974; Hook *et al.*, 1994). The remaining structures adopt the usual motif for $R_2Sn(S_2CNR'R'')_2$, namely a geometry based on a bipyramidal skewed-bipyramid. Here, the dithiocarbamate ligands coordinate in an asymmetric fashion with the tin-bound phenyl substituents disposed to lie over the weaker Sn—S bonds, exemplified by the two independent molecules comprising the asymmetric unit of $Ph_2Sn[S_2CN(Me)Hex]_2$ (Hex = *n*-hexyl, –$C_7H_{15}$) (Ramasamy *et al.*, 2013). Clearly there is a subtle interplay between the electronic and steric characteristics of the dithiocarbamate ligands and molecular packing effects in determining the structural motif adopted by $Ph_2Sn(S_2CNR'R'')_2$ in their respective crystals.

## 7. Synthesis and crystallization

All chemicals and solvents were used as purchased without purification. The melting point was determined using an automated melting point apparatus (MPA 120 EZ-Melt). Carbon, hydrogen and nitrogen analyses were performed on a Leco CHNS-932 Elemental Analyzer.

The synthesis of (I) and (II) followed established literature procedures (Awang *et al.*, 2011; Ajibade *et al.*, 2011). For each synthesis, initially, diallylamine (Aldrich; 1.27 ml, 10 mmol) dissolved in ethanol (30 ml) was stirred under ice-bath conditions for 20 mins. A 25% ammonia solution (1 to 2 ml) was added followed by stirring for 30 mins to establish basic conditions. Then, a cold ethanolic solution of carbon disulfide (0.60 ml, 10 mmol) was added dropwise into the solution and stirred for about 2 h.

For (I), triphenyltin(IV) dichloride (Merck; 3.85 g, 10 mmol) dissolved in ethanol (20–30 ml) was added dropwise into the diallyldithiocarbamate solution and further stirred for 2 to 3 h. Next, the precipitate that formed was filtered off and washed with cold ethanol a few times to remove any impurities. Finally, the filtered precipitate was dried in a desiccator overnight. Recrystallization was carried out by dissolving the

**Table 8**
Experimental details.

| | (I) | (II) |
|---|---|---|
| Crystal data | | |
| Chemical formula | $[Sn(C_6H_5)_3(C_7H_{10}NS_2)]$ | $[Sn(C_6H_5)_2(C_7H_{10}NS_2)_2]$ |
| $M_r$ | 522.27 | 617.45 |
| Crystal system, space group | Monoclinic, $P2_1/c$ | Monoclinic, $P2_1/c$ |
| Temperature (K) | 100 | 100 |
| $a, b, c$ (Å) | 8.0650 (1), 11.4490 (1), 25.8775 (2) | 9.6160 (1), 30.4216 (2), 19.1928 (1) |
| $\beta$ (°) | 98.282 (1) | 100.019 (1) |
| $V$ (Å$^3$) | 2364.51 (4) | 5528.93 (8) |
| $Z$ | 4 | 8 |
| Radiation type | Cu $K\alpha$ | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 10.32 | 10.30 |
| Crystal size (mm) | 0.13 × 0.10 × 0.04 | 0.19 × 0.14 × 0.07 |
| Data collection | | |
| Diffractometer | XtaLAB Synergy, Dualflex, AtlasS2 | XtaLAB Synergy, Dualflex, AtlasS2 |
| Absorption correction | Gaussian (*CrysAlis PRO*; Rigaku OD, 2018) | Gaussian (*CrysAlis PRO*; Rigaku OD, 2018) |
| $T_{min}$, $T_{max}$ | 0.807, 1.000 | 0.633, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 55086, 4226, 4083 | 67735, 9876, 9370 |
| $R_{int}$ | 0.044 | 0.037 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.597 | 0.597 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.020, 0.053, 1.01 | 0.027, 0.068, 1.02 |
| No. of reflections | 4226 | 9876 |
| No. of parameters | 262 | 595 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.82, −0.50 | 1.23, −0.73 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXS* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

compound in a chloroform and ethanol solvent mixture (5 ml; 1:1 *v*/*v*), which was allowed to slowly evaporate at room temperature yielding colourless crystals. Yield: 44%. M.p. 454.8–456.2 K. Elemental analysis: calculated (%): C 57.51, H 4.79, N 2.68. Found (%): C 56.92, H 4.93, N 2.93.

Compound (II) was prepared and recrystallized as for (I) but, using diphenyltin(IV) dichloride (Merck; 1.72 g, 5 mmol) dissolved in ethanol (20-30 ml). Yield: 52%. M.p. 332.5–334.4 K. Elemental analysis: calculated (%): C 50.59, H 4.86, N 4.54. Found (%): C 50.20, H 4.80, N 4.20.

## 8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 8. 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 $U_{iso}$(H) set to 1.2$U_{eq}$(C). In (II), the maximum and minimum residual electron density peaks of 1.23 and 0.73 e Å$^{-3}$, respectively, were located 0.80 and 0.74 Å from the S2 and Sn1 atoms, respectively.

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# supporting information

*Acta Cryst.* (2020). E**76**, 167-176 [https://doi.org/10.1107/S2056989020000122]

## (*N*,*N*-Diallyldithiocarbamato-$\kappa^2S,S'$)triphenyltin(IV) and bis(*N*,*N*-diallyldithiocarbamato-$\kappa^2S,S'$)diphenyltin(IV): crystal structure, Hirshfeld surface analysis and computational study

**Farah Natasha Haezam, Normah Awang, Nurul Farahana Kamaludin, Mukesh M. Jotani and Edward R. T. Tiekink**

### Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SHELXS* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### (*N*,*N*-Diallyldithiocarbamato-$\kappa^2S,S'$)\ triphenyltin(IV) (I)

*Crystal data*

$[Sn(C_6H_5)_3(C_7H_{10}NS_2)]$
$M_r$ = 522.27
Monoclinic, $P2_1/c$
$a$ = 8.0650 (1) Å
$b$ = 11.4490 (1) Å
$c$ = 25.8775 (2) Å
$\beta$ = 98.282 (1)°
$V$ = 2364.51 (4) Å$^3$
$Z$ = 4
$F(000)$ = 1056
$D_x$ = 1.467 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 34049 reflections
$\theta$ = 3.4–76.3°
$\mu$ = 10.32 mm$^{-1}$
$T$ = 100 K
Prism, colourless
0.13 × 0.10 × 0.04 mm

*Data collection*

XtaLAB Synergy, Dualflex, AtlasS2 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.2558 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2018)
$T_{min}$ = 0.807, $T_{max}$ = 1.000
55086 measured reflections
4226 independent reflections
4083 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044
$\theta_{max}$ = 67.1°, $\theta_{min}$ = 3.5°
$h$ = −9→9
$k$ = −13→13
$l$ = −26→30

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.053$
$S = 1.01$
4226 reflections
262 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
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.0941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å$^{-3}$
$\Delta\rho_{min} = -0.50$ e Å$^{-3}$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn | 0.25851 (2) | 0.27508 (2) | 0.37027 (2) | 0.01943 (6) |
| S1 | 0.40753 (6) | 0.34500 (4) | 0.45492 (2) | 0.02546 (11) |
| S2 | 0.50865 (6) | 0.11062 (4) | 0.42287 (2) | 0.02585 (11) |
| N1 | 0.6650 (2) | 0.22704 (13) | 0.50510 (7) | 0.0221 (3) |
| C1 | 0.5424 (2) | 0.22413 (16) | 0.46477 (8) | 0.0211 (4) |
| C2 | 0.6883 (2) | 0.32426 (18) | 0.54246 (8) | 0.0267 (4) |
| H2A | 0.646687 | 0.397215 | 0.524565 | 0.032* |
| H2B | 0.809419 | 0.334224 | 0.554922 | 0.032* |
| C3 | 0.5978 (3) | 0.3042 (2) | 0.58847 (8) | 0.0309 (5) |
| H3 | 0.612847 | 0.360684 | 0.615638 | 0.037* |
| C4 | 0.4992 (3) | 0.2149 (2) | 0.59435 (9) | 0.0319 (5) |
| H4A | 0.480682 | 0.156449 | 0.568121 | 0.038* |
| H4B | 0.446654 | 0.209057 | 0.624828 | 0.038* |
| C5 | 0.7846 (2) | 0.12945 (18) | 0.51605 (8) | 0.0249 (4) |
| H5A | 0.732148 | 0.056406 | 0.501157 | 0.030* |
| H5B | 0.812801 | 0.118925 | 0.554284 | 0.030* |
| C6 | 0.9410 (3) | 0.1527 (2) | 0.49311 (9) | 0.0315 (4) |
| H6 | 0.931935 | 0.161093 | 0.456289 | 0.038* |
| C7 | 1.0904 (3) | 0.1621 (2) | 0.52078 (11) | 0.0427 (6) |
| H7A | 1.103510 | 0.154114 | 0.557684 | 0.051* |
| H7B | 1.185305 | 0.176968 | 0.503870 | 0.051* |
| C11 | 0.0883 (2) | 0.13134 (16) | 0.35523 (7) | 0.0204 (4) |
| C12 | −0.0823 (2) | 0.15586 (18) | 0.34399 (7) | 0.0257 (4) |
| H12 | −0.120299 | 0.233677 | 0.347295 | 0.031* |
| C13 | −0.1979 (2) | 0.06837 (19) | 0.32802 (8) | 0.0278 (4) |
| H13 | −0.313765 | 0.086573 | 0.320597 | 0.033* |
| C14 | −0.1442 (3) | −0.04484 (19) | 0.32295 (8) | 0.0279 (4) |
| H14 | −0.222732 | −0.104752 | 0.311737 | 0.033* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.0259 (3) | −0.07077 (18) | 0.33438 (9) | 0.0308 (4) |
| H15 | 0.063245 | −0.148801 | 0.331218 | 0.037* |
| C16 | 0.1410 (2) | 0.01651 (17) | 0.35033 (8) | 0.0254 (4) |
| H16 | 0.256747 | −0.002093 | 0.357990 | 0.030* |
| C21 | 0.4161 (2) | 0.28918 (16) | 0.31120 (7) | 0.0213 (4) |
| C22 | 0.5403 (2) | 0.37446 (18) | 0.31258 (8) | 0.0269 (4) |
| H22 | 0.554696 | 0.429581 | 0.340305 | 0.032* |
| C23 | 0.6428 (3) | 0.37983 (19) | 0.27407 (9) | 0.0312 (5) |
| H23 | 0.726432 | 0.438594 | 0.275407 | 0.037* |
| C24 | 0.6234 (3) | 0.2996 (2) | 0.23361 (9) | 0.0313 (5) |
| H24 | 0.693634 | 0.303209 | 0.207178 | 0.038* |
| C25 | 0.5010 (3) | 0.21372 (18) | 0.23174 (8) | 0.0280 (4) |
| H25 | 0.487954 | 0.158250 | 0.204148 | 0.034* |
| C26 | 0.3979 (2) | 0.20907 (17) | 0.27018 (8) | 0.0223 (4) |
| H26 | 0.313726 | 0.150577 | 0.268562 | 0.027* |
| C31 | 0.0978 (2) | 0.42764 (17) | 0.36369 (8) | 0.0242 (4) |
| C32 | −0.0065 (3) | 0.45310 (18) | 0.40077 (8) | 0.0293 (4) |
| H32 | −0.007314 | 0.402694 | 0.429894 | 0.035* |
| C33 | −0.1095 (3) | 0.5512 (2) | 0.39575 (10) | 0.0357 (5) |
| H33 | −0.180213 | 0.567475 | 0.421210 | 0.043* |
| C34 | −0.1081 (3) | 0.62513 (19) | 0.35328 (10) | 0.0374 (5) |
| H34 | −0.177793 | 0.692406 | 0.349818 | 0.045* |
| C35 | −0.0067 (3) | 0.60157 (19) | 0.31626 (9) | 0.0350 (5) |
| H35 | −0.006485 | 0.652566 | 0.287313 | 0.042* |
| C36 | 0.0959 (2) | 0.50318 (18) | 0.32102 (8) | 0.0273 (4) |
| H36 | 0.165193 | 0.487164 | 0.295126 | 0.033* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn | 0.02063 (8) | 0.01640 (8) | 0.02001 (8) | 0.00251 (4) | −0.00135 (5) | −0.00007 (4) |
| S1 | 0.0271 (2) | 0.0215 (2) | 0.0253 (2) | 0.00683 (18) | −0.00475 (18) | −0.00472 (17) |
| S2 | 0.0301 (2) | 0.0205 (2) | 0.0254 (2) | 0.00408 (18) | −0.00133 (18) | −0.00396 (18) |
| N1 | 0.0206 (8) | 0.0200 (9) | 0.0246 (8) | 0.0016 (6) | −0.0007 (7) | 0.0000 (6) |
| C1 | 0.0186 (9) | 0.0212 (10) | 0.0232 (9) | 0.0002 (7) | 0.0025 (7) | 0.0024 (7) |
| C2 | 0.0249 (10) | 0.0223 (10) | 0.0303 (10) | −0.0022 (8) | −0.0051 (8) | −0.0028 (8) |
| C3 | 0.0314 (11) | 0.0333 (11) | 0.0255 (10) | 0.0014 (9) | −0.0043 (8) | −0.0109 (9) |
| C4 | 0.0289 (11) | 0.0404 (13) | 0.0257 (10) | 0.0021 (9) | 0.0015 (8) | −0.0050 (8) |
| C5 | 0.0215 (9) | 0.0240 (10) | 0.0282 (10) | 0.0029 (8) | 0.0005 (7) | 0.0037 (8) |
| C6 | 0.0285 (10) | 0.0312 (11) | 0.0356 (11) | 0.0057 (9) | 0.0074 (9) | 0.0036 (9) |
| C7 | 0.0255 (11) | 0.0398 (14) | 0.0632 (16) | 0.0002 (10) | 0.0083 (10) | 0.0010 (12) |
| C11 | 0.0245 (9) | 0.0192 (9) | 0.0173 (8) | 0.0018 (7) | 0.0029 (7) | 0.0011 (7) |
| C12 | 0.0245 (9) | 0.0241 (10) | 0.0270 (9) | 0.0061 (8) | −0.0013 (8) | −0.0026 (8) |
| C13 | 0.0212 (9) | 0.0328 (11) | 0.0279 (10) | 0.0015 (8) | −0.0011 (7) | 0.0008 (8) |
| C14 | 0.0278 (10) | 0.0268 (11) | 0.0296 (10) | −0.0080 (8) | 0.0059 (8) | −0.0019 (8) |
| C15 | 0.0298 (10) | 0.0187 (10) | 0.0453 (12) | −0.0004 (8) | 0.0107 (9) | −0.0025 (9) |
| C16 | 0.0233 (9) | 0.0190 (10) | 0.0347 (10) | 0.0017 (8) | 0.0069 (8) | −0.0005 (8) |
| C21 | 0.0203 (9) | 0.0204 (9) | 0.0215 (9) | 0.0019 (7) | −0.0024 (7) | 0.0036 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C22 | 0.0260 (10) | 0.0203 (10) | 0.0320 (10) | −0.0032 (8) | −0.0037 (8) | 0.0013 (8) |
| C23 | 0.0235 (10) | 0.0288 (11) | 0.0396 (11) | −0.0078 (8) | −0.0012 (8) | 0.0090 (9) |
| C24 | 0.0230 (10) | 0.0387 (12) | 0.0325 (11) | −0.0006 (9) | 0.0051 (8) | 0.0097 (9) |
| C25 | 0.0276 (10) | 0.0297 (11) | 0.0258 (10) | −0.0019 (8) | 0.0006 (8) | 0.0010 (8) |
| C26 | 0.0206 (9) | 0.0224 (9) | 0.0227 (9) | −0.0032 (7) | −0.0004 (7) | 0.0022 (7) |
| C31 | 0.0226 (9) | 0.0154 (9) | 0.0318 (10) | 0.0013 (7) | −0.0053 (8) | −0.0033 (7) |
| C32 | 0.0284 (10) | 0.0207 (10) | 0.0366 (11) | 0.0016 (8) | −0.0022 (8) | −0.0044 (8) |
| C33 | 0.0245 (10) | 0.0270 (11) | 0.0534 (13) | 0.0010 (9) | −0.0018 (9) | −0.0144 (10) |
| C34 | 0.0263 (10) | 0.0179 (10) | 0.0621 (15) | 0.0029 (8) | −0.0139 (10) | −0.0059 (10) |
| C35 | 0.0306 (11) | 0.0205 (10) | 0.0481 (13) | −0.0019 (9) | −0.0140 (10) | 0.0033 (9) |
| C36 | 0.0247 (9) | 0.0201 (10) | 0.0331 (10) | −0.0016 (8) | −0.0099 (8) | −0.0001 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Sn—C21 | 2.130 (2) | C13—H13 | 0.9500 |
| Sn—C11 | 2.1427 (19) | C14—C15 | 1.393 (3) |
| Sn—C31 | 2.1673 (19) | C14—H14 | 0.9500 |
| Sn—S1 | 2.4749 (4) | C15—C16 | 1.386 (3) |
| Sn—S2 | 2.9456 (5) | C15—H15 | 0.9500 |
| S1—C1 | 1.7559 (19) | C16—H16 | 0.9500 |
| S2—C1 | 1.6894 (19) | C21—C26 | 1.394 (3) |
| N1—C1 | 1.330 (3) | C21—C22 | 1.395 (3) |
| N1—C2 | 1.468 (3) | C22—C23 | 1.384 (3) |
| N1—C5 | 1.477 (2) | C22—H22 | 0.9500 |
| C2—C3 | 1.502 (3) | C23—C24 | 1.385 (3) |
| C2—H2A | 0.9900 | C23—H23 | 0.9500 |
| C2—H2B | 0.9900 | C24—C25 | 1.388 (3) |
| C3—C4 | 1.317 (3) | C24—H24 | 0.9500 |
| C3—H3 | 0.9500 | C25—C26 | 1.387 (3) |
| C4—H4A | 0.9500 | C25—H25 | 0.9500 |
| C4—H4B | 0.9500 | C26—H26 | 0.9500 |
| C5—C6 | 1.493 (3) | C31—C32 | 1.395 (3) |
| C5—H5A | 0.9900 | C31—C36 | 1.401 (3) |
| C5—H5B | 0.9900 | C32—C33 | 1.392 (3) |
| C6—C7 | 1.315 (3) | C32—H32 | 0.9500 |
| C6—H6 | 0.9500 | C33—C34 | 1.388 (4) |
| C7—H7A | 0.9500 | C33—H33 | 0.9500 |
| C7—H7B | 0.9500 | C34—C35 | 1.373 (4) |
| C11—C12 | 1.393 (3) | C34—H34 | 0.9500 |
| C11—C16 | 1.393 (3) | C35—C36 | 1.393 (3) |
| C12—C13 | 1.390 (3) | C35—H35 | 0.9500 |
| C12—H12 | 0.9500 | C36—H36 | 0.9500 |
| C13—C14 | 1.379 (3) | | |

| | | | |
|---|---|---|---|
| C21—Sn—C11 | 111.15 (7) | C14—C13—C12 | 119.99 (18) |
| C21—Sn—C31 | 107.13 (7) | C14—C13—H13 | 120.0 |
| C11—Sn—C31 | 104.14 (7) | C12—C13—H13 | 120.0 |
| C21—Sn—S1 | 110.28 (5) | C13—C14—C15 | 119.53 (19) |

| | | | |
|---|---|---|---|
| C11—Sn—S1 | 128.76 (5) | C13—C14—H14 | 120.2 |
| C31—Sn—S1 | 91.01 (5) | C15—C14—H14 | 120.2 |
| C21—Sn—S2 | 86.57 (5) | C16—C15—C14 | 120.43 (19) |
| C11—Sn—S2 | 88.36 (5) | C16—C15—H15 | 119.8 |
| C31—Sn—S2 | 156.01 (5) | C14—C15—H15 | 119.8 |
| S1—Sn—S2 | 65.470 (14) | C15—C16—C11 | 120.48 (18) |
| C1—S1—Sn | 94.89 (7) | C15—C16—H16 | 119.8 |
| C1—S2—Sn | 80.86 (6) | C11—C16—H16 | 119.8 |
| C1—N1—C2 | 123.08 (16) | C26—C21—C22 | 118.46 (19) |
| C1—N1—C5 | 121.51 (16) | C26—C21—Sn | 119.19 (14) |
| C2—N1—C5 | 115.39 (15) | C22—C21—Sn | 122.33 (15) |
| N1—C1—S2 | 123.75 (14) | C23—C22—C21 | 120.87 (19) |
| N1—C1—S1 | 117.96 (14) | C23—C22—H22 | 119.6 |
| S2—C1—S1 | 118.29 (11) | C21—C22—H22 | 119.6 |
| N1—C2—C3 | 112.04 (17) | C22—C23—C24 | 120.03 (19) |
| N1—C2—H2A | 109.2 | C22—C23—H23 | 120.0 |
| C3—C2—H2A | 109.2 | C24—C23—H23 | 120.0 |
| N1—C2—H2B | 109.2 | C23—C24—C25 | 119.9 (2) |
| C3—C2—H2B | 109.2 | C23—C24—H24 | 120.1 |
| H2A—C2—H2B | 107.9 | C25—C24—H24 | 120.1 |
| C4—C3—C2 | 125.52 (19) | C26—C25—C24 | 119.9 (2) |
| C4—C3—H3 | 117.2 | C26—C25—H25 | 120.0 |
| C2—C3—H3 | 117.2 | C24—C25—H25 | 120.0 |
| C3—C4—H4A | 120.0 | C25—C26—C21 | 120.81 (18) |
| C3—C4—H4B | 120.0 | C25—C26—H26 | 119.6 |
| H4A—C4—H4B | 120.0 | C21—C26—H26 | 119.6 |
| N1—C5—C6 | 110.80 (17) | C32—C31—C36 | 118.31 (19) |
| N1—C5—H5A | 109.5 | C32—C31—Sn | 121.84 (15) |
| C6—C5—H5A | 109.5 | C36—C31—Sn | 119.85 (15) |
| N1—C5—H5B | 109.5 | C31—C32—C33 | 121.0 (2) |
| C6—C5—H5B | 109.5 | C31—C32—H32 | 119.5 |
| H5A—C5—H5B | 108.1 | C33—C32—H32 | 119.5 |
| C7—C6—C5 | 124.0 (2) | C34—C33—C32 | 119.6 (2) |
| C7—C6—H6 | 118.0 | C34—C33—H33 | 120.2 |
| C5—C6—H6 | 118.0 | C32—C33—H33 | 120.2 |
| C6—C7—H7A | 120.0 | C35—C34—C33 | 120.4 (2) |
| C6—C7—H7B | 120.0 | C35—C34—H34 | 119.8 |
| H7A—C7—H7B | 120.0 | C33—C34—H34 | 119.8 |
| C12—C11—C16 | 118.46 (18) | C34—C35—C36 | 120.2 (2) |
| C12—C11—Sn | 118.09 (14) | C34—C35—H35 | 119.9 |
| C16—C11—Sn | 123.03 (14) | C36—C35—H35 | 119.9 |
| C13—C12—C11 | 121.09 (19) | C35—C36—C31 | 120.5 (2) |
| C13—C12—H12 | 119.5 | C35—C36—H36 | 119.7 |
| C11—C12—H12 | 119.5 | C31—C36—H36 | 119.7 |
| | | | |
| C2—N1—C1—S2 | −177.36 (15) | C14—C15—C16—C11 | 0.1 (3) |
| C5—N1—C1—S2 | 0.8 (3) | C12—C11—C16—C15 | 0.3 (3) |
| C2—N1—C1—S1 | 2.3 (3) | Sn—C11—C16—C15 | −172.13 (15) |

| | | | |
|---|---|---|---|
| C5—N1—C1—S1 | −179.62 (14) | C26—C21—C22—C23 | 0.2 (3) |
| Sn—S2—C1—N1 | −174.18 (18) | Sn—C21—C22—C23 | 178.75 (15) |
| Sn—S2—C1—S1 | 6.21 (10) | C21—C22—C23—C24 | −0.3 (3) |
| Sn—S1—C1—N1 | 173.04 (15) | C22—C23—C24—C25 | 0.0 (3) |
| Sn—S1—C1—S2 | −7.33 (12) | C23—C24—C25—C26 | 0.4 (3) |
| C1—N1—C2—C3 | 91.6 (2) | C24—C25—C26—C21 | −0.5 (3) |
| C5—N1—C2—C3 | −86.6 (2) | C22—C21—C26—C25 | 0.2 (3) |
| N1—C2—C3—C4 | −4.2 (3) | Sn—C21—C26—C25 | −178.38 (15) |
| C1—N1—C5—C6 | 95.9 (2) | C36—C31—C32—C33 | −0.3 (3) |
| C2—N1—C5—C6 | −85.9 (2) | Sn—C31—C32—C33 | −179.70 (14) |
| N1—C5—C6—C7 | 118.2 (2) | C31—C32—C33—C34 | −0.2 (3) |
| C16—C11—C12—C13 | −0.3 (3) | C32—C33—C34—C35 | 0.3 (3) |
| Sn—C11—C12—C13 | 172.55 (15) | C33—C34—C35—C36 | 0.0 (3) |
| C11—C12—C13—C14 | −0.2 (3) | C34—C35—C36—C31 | −0.4 (3) |
| C12—C13—C14—C15 | 0.6 (3) | C32—C31—C36—C35 | 0.6 (3) |
| C13—C14—C15—C16 | −0.5 (3) | Sn—C31—C36—C35 | −179.98 (14) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 and *Cg*2 are the centroids of the (C21–C26) and (C31–C36) rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13···*Cg*1$^{i}$ | 0.95 | 2.92 | 3.605 (2) | 130 |
| C23—H23···*Cg*2$^{ii}$ | 0.95 | 2.99 | 3.720 (3) | 134 |

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

## Bis(*N*,*N*-diallyldithiocarbamato-$\kappa^2S,S'$)diphenyltin(IV) (II)

*Crystal data*

| | |
|---|---|
| $[Sn(C_6H_5)_2(C_7H_{10}NS_2)_2]$ | $F(000)$ = 2512 |
| $M_r$ = 617.45 | $D_x$ = 1.484 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å |
| $a$ = 9.6160 (1) Å | Cell parameters from 40535 reflections |
| $b$ = 30.4216 (2) Å | $\theta$ = 2.9–76.3° |
| $c$ = 19.1928 (1) Å | $\mu$ = 10.30 mm$^{-1}$ |
| $\beta$ = 100.019 (1)° | $T$ = 100 K |
| $V$ = 5528.93 (8) Å$^3$ | Prism, colourless |
| $Z$ = 8 | 0.19 × 0.14 × 0.07 mm |

*Data collection*

| | |
|---|---|
| XtaLAB Synergy, Dualflex, AtlasS2 diffractometer | $T_{min}$ = 0.633, $T_{max}$ = 1.000 |
| Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source | 67735 measured reflections |
| Mirror monochromator | 9876 independent reflections |
| Detector resolution: 5.2558 pixels mm$^{-1}$ | 9370 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int}$ = 0.037 |
| Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2018) | $\theta_{max}$ = 67.1°, $\theta_{min}$ = 3.7° |
| | $h$ = −11→11 |
| | $k$ = −36→25 |
| | $l$ = −22→22 |

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.068$
$S = 1.01$
9876 reflections
595 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
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 7.0312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.73$ e Å$^{-3}$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | 0.96840 (2) | 0.26758 (2) | 0.60783 (2) | 0.01863 (5) |
| S1 | 1.05093 (7) | 0.34237 (2) | 0.65910 (3) | 0.02202 (13) |
| S2 | 1.05034 (7) | 0.32188 (2) | 0.50854 (3) | 0.02481 (13) |
| S3 | 0.82312 (7) | 0.21606 (2) | 0.51668 (4) | 0.02761 (14) |
| S4 | 0.71629 (7) | 0.30174 (2) | 0.55382 (3) | 0.02345 (13) |
| N1 | 1.1264 (2) | 0.39971 (7) | 0.56894 (11) | 0.0203 (4) |
| N2 | 0.5656 (2) | 0.24617 (7) | 0.46333 (12) | 0.0253 (5) |
| C1 | 1.0824 (2) | 0.35895 (8) | 0.57638 (13) | 0.0189 (5) |
| C2 | 1.1517 (3) | 0.41701 (9) | 0.50102 (14) | 0.0251 (6) |
| H2A | 1.121986 | 0.448186 | 0.496767 | 0.030* |
| H2B | 1.093159 | 0.400473 | 0.462164 | 0.030* |
| C3 | 1.3039 (3) | 0.41377 (9) | 0.49308 (14) | 0.0286 (6) |
| H3 | 1.331520 | 0.429629 | 0.455081 | 0.034* |
| C4 | 1.4027 (3) | 0.39104 (10) | 0.53379 (16) | 0.0309 (6) |
| H4A | 1.380189 | 0.374657 | 0.572463 | 0.037* |
| H4B | 1.496585 | 0.391033 | 0.524485 | 0.037* |
| C5 | 1.1518 (3) | 0.43140 (8) | 0.62834 (14) | 0.0225 (5) |
| H5A | 1.229774 | 0.451427 | 0.621918 | 0.027* |
| H5B | 1.180874 | 0.415255 | 0.673303 | 0.027* |
| C6 | 1.0221 (3) | 0.45784 (9) | 0.63244 (13) | 0.0246 (5) |
| H6 | 0.938442 | 0.442486 | 0.637625 | 0.030* |
| C7 | 1.0169 (3) | 0.50095 (10) | 0.62931 (15) | 0.0312 (6) |
| H7A | 1.098766 | 0.517238 | 0.624141 | 0.037* |
| H7B | 0.931250 | 0.515847 | 0.632218 | 0.037* |
| C8 | 0.6860 (3) | 0.25402 (8) | 0.50603 (13) | 0.0211 (5) |
| C9 | 0.4473 (3) | 0.27826 (9) | 0.45194 (15) | 0.0270 (6) |
| H9A | 0.459611 | 0.299926 | 0.491021 | 0.032* |
| H9B | 0.356671 | 0.262729 | 0.451561 | 0.032* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.4444 (3) | 0.30145 (11) | 0.38295 (16) | 0.0357 (7) |
| H10 | 0.513805 | 0.323315 | 0.380204 | 0.043* |
| C11 | 0.3516 (4) | 0.29318 (13) | 0.32636 (18) | 0.0485 (9) |
| H11A | 0.281054 | 0.271475 | 0.327679 | 0.058* |
| H11B | 0.354463 | 0.308876 | 0.283842 | 0.058* |
| C12 | 0.5396 (3) | 0.20533 (10) | 0.42143 (16) | 0.0341 (7) |
| H12A | 0.630727 | 0.190610 | 0.419544 | 0.041* |
| H12B | 0.494638 | 0.212628 | 0.372403 | 0.041* |
| C13 | 0.4460 (4) | 0.17484 (10) | 0.45334 (18) | 0.0415 (8) |
| H13 | 0.483016 | 0.161495 | 0.497427 | 0.050* |
| C14 | 0.3162 (4) | 0.16547 (13) | 0.4240 (3) | 0.0601 (11) |
| H14A | 0.276367 | 0.178312 | 0.379956 | 0.072* |
| H14B | 0.261771 | 0.145828 | 0.446853 | 0.072* |
| C15 | 1.1604 (3) | 0.22965 (8) | 0.61670 (13) | 0.0210 (5) |
| C16 | 1.2902 (3) | 0.24774 (9) | 0.60881 (14) | 0.0247 (5) |
| H16 | 1.295812 | 0.277867 | 0.596567 | 0.030* |
| C17 | 1.4111 (3) | 0.22188 (9) | 0.61878 (16) | 0.0289 (6) |
| H17 | 1.499314 | 0.234539 | 0.614001 | 0.035* |
| C18 | 1.4039 (3) | 0.17786 (9) | 0.63562 (14) | 0.0273 (6) |
| H18 | 1.486760 | 0.160247 | 0.641839 | 0.033* |
| C19 | 1.2754 (3) | 0.15942 (9) | 0.64342 (14) | 0.0256 (6) |
| H19 | 1.270001 | 0.129177 | 0.654966 | 0.031* |
| C20 | 1.1552 (3) | 0.18534 (9) | 0.63427 (13) | 0.0230 (5) |
| H20 | 1.067687 | 0.172668 | 0.640090 | 0.028* |
| C21 | 0.8975 (3) | 0.24718 (8) | 0.70441 (13) | 0.0203 (5) |
| C22 | 0.9742 (3) | 0.26067 (9) | 0.76923 (14) | 0.0265 (6) |
| H22 | 1.055704 | 0.278445 | 0.770037 | 0.032* |
| C23 | 0.9342 (3) | 0.24871 (10) | 0.83264 (15) | 0.0323 (6) |
| H23 | 0.988359 | 0.258258 | 0.876175 | 0.039* |
| C24 | 0.8158 (3) | 0.22295 (10) | 0.83270 (16) | 0.0317 (6) |
| H24 | 0.787943 | 0.214921 | 0.876082 | 0.038* |
| C25 | 0.7383 (3) | 0.20897 (10) | 0.76898 (16) | 0.0327 (6) |
| H25 | 0.656701 | 0.191282 | 0.768520 | 0.039* |
| C26 | 0.7797 (3) | 0.22080 (9) | 0.70546 (15) | 0.0266 (6) |
| H26 | 0.726533 | 0.210653 | 0.662062 | 0.032* |
| Sn2 | 0.42934 (2) | 0.47935 (2) | 0.26224 (2) | 0.01967 (5) |
| S1A | 0.50653 (7) | 0.43729 (2) | 0.15999 (3) | 0.02630 (14) |
| S2A | 0.65505 (7) | 0.51843 (2) | 0.21454 (3) | 0.02630 (14) |
| S3A | 0.39019 (7) | 0.55322 (2) | 0.32085 (3) | 0.02589 (14) |
| S4A | 0.29651 (7) | 0.53675 (2) | 0.16787 (3) | 0.02586 (14) |
| N1A | 0.6984 (2) | 0.47703 (7) | 0.09775 (12) | 0.0264 (5) |
| N2A | 0.2774 (2) | 0.61450 (7) | 0.22935 (11) | 0.0229 (4) |
| C1A | 0.6292 (3) | 0.47819 (8) | 0.15187 (14) | 0.0234 (5) |
| C2A | 0.6696 (3) | 0.44435 (10) | 0.03990 (15) | 0.0328 (6) |
| H2A1 | 0.675651 | 0.458786 | −0.005706 | 0.039* |
| H2A2 | 0.572710 | 0.432678 | 0.037076 | 0.039* |
| C3A | 0.7733 (4) | 0.40729 (10) | 0.05215 (16) | 0.0375 (7) |
| H3A | 0.763123 | 0.386079 | 0.087245 | 0.045* |

| | | | | |
|---|---|---|---|---|
| C4A | 0.8781 (4) | 0.40263 (11) | 0.01660 (17) | 0.0400 (7) |
| H4A1 | 0.890527 | 0.423401 | −0.018758 | 0.048* |
| H4A2 | 0.941186 | 0.378490 | 0.026373 | 0.048* |
| C5A | 0.8112 (3) | 0.50881 (10) | 0.09071 (15) | 0.0280 (6) |
| H5A1 | 0.888230 | 0.493556 | 0.072253 | 0.034* |
| H5A2 | 0.850815 | 0.520988 | 0.137826 | 0.034* |
| C6A | 0.7561 (4) | 0.54519 (12) | 0.04217 (19) | 0.0446 (8) |
| H6A | 0.688042 | 0.564544 | 0.055802 | 0.053* |
| C7A | 0.7971 (5) | 0.55184 (17) | −0.0189 (2) | 0.0720 (15) |
| H7A1 | 0.865062 | 0.532902 | −0.033670 | 0.086* |
| H7A2 | 0.758874 | 0.575581 | −0.048313 | 0.086* |
| C8A | 0.3158 (3) | 0.57268 (8) | 0.23782 (13) | 0.0221 (5) |
| C9A | 0.2113 (3) | 0.63244 (9) | 0.16070 (14) | 0.0254 (6) |
| H9A1 | 0.250124 | 0.617093 | 0.122830 | 0.030* |
| H9A2 | 0.236138 | 0.663945 | 0.158775 | 0.030* |
| C10A | 0.0529 (3) | 0.62794 (9) | 0.14665 (14) | 0.0270 (6) |
| H10A | 0.003035 | 0.643092 | 0.106705 | 0.032* |
| C11A | −0.0226 (3) | 0.60500 (9) | 0.18449 (15) | 0.0296 (6) |
| H11C | 0.022624 | 0.589294 | 0.224927 | 0.036* |
| H11D | −0.122521 | 0.604126 | 0.171420 | 0.036* |
| C12A | 0.3060 (3) | 0.64644 (9) | 0.28729 (15) | 0.0262 (6) |
| H12C | 0.306030 | 0.631114 | 0.332786 | 0.031* |
| H12D | 0.229511 | 0.668611 | 0.281445 | 0.031* |
| C13A | 0.4451 (3) | 0.66935 (9) | 0.28974 (15) | 0.0304 (6) |
| H13A | 0.461271 | 0.694727 | 0.318873 | 0.036* |
| C14A | 0.5464 (3) | 0.65786 (11) | 0.25573 (16) | 0.0345 (7) |
| H14C | 0.535363 | 0.632722 | 0.225908 | 0.041* |
| H14D | 0.630812 | 0.674669 | 0.260903 | 0.041* |
| C15A | 0.5755 (3) | 0.45369 (8) | 0.35224 (13) | 0.0199 (5) |
| C16A | 0.6517 (3) | 0.41536 (9) | 0.34627 (15) | 0.0262 (6) |
| H16A | 0.641902 | 0.400827 | 0.301871 | 0.031* |
| C17A | 0.7420 (3) | 0.39798 (9) | 0.40436 (16) | 0.0281 (6) |
| H17A | 0.792462 | 0.371612 | 0.399584 | 0.034* |
| C18A | 0.7580 (3) | 0.41916 (9) | 0.46894 (15) | 0.0267 (6) |
| H18A | 0.819483 | 0.407280 | 0.508595 | 0.032* |
| C19A | 0.6849 (3) | 0.45768 (9) | 0.47610 (14) | 0.0263 (6) |
| H19A | 0.696848 | 0.472399 | 0.520395 | 0.032* |
| C20A | 0.5935 (3) | 0.47474 (9) | 0.41787 (14) | 0.0222 (5) |
| H20A | 0.542863 | 0.501025 | 0.422959 | 0.027* |
| C21A | 0.2380 (3) | 0.44192 (9) | 0.26420 (13) | 0.0219 (5) |
| C22A | 0.2467 (3) | 0.40539 (9) | 0.30792 (14) | 0.0263 (6) |
| H22A | 0.335183 | 0.397555 | 0.335339 | 0.032* |
| C23A | 0.1275 (3) | 0.37983 (10) | 0.31248 (16) | 0.0322 (6) |
| H23A | 0.135091 | 0.355207 | 0.343351 | 0.039* |
| C24A | −0.0010 (3) | 0.39055 (10) | 0.27192 (16) | 0.0330 (6) |
| H24A | −0.082123 | 0.373216 | 0.274518 | 0.040* |
| C25A | −0.0111 (3) | 0.42636 (11) | 0.22781 (17) | 0.0387 (7) |
| H25A | −0.099646 | 0.433692 | 0.199882 | 0.046* |

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|---|---|---|---|---|
| C26A | 0.1072 (3) | 0.45212 (10) | 0.22356 (16) | 0.0333 (6) |
| H26A | 0.098571 | 0.476793 | 0.192762 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn1 | 0.01673 (9) | 0.01771 (9) | 0.02066 (9) | 0.00008 (6) | 0.00108 (6) | 0.00380 (6) |
| S1 | 0.0246 (3) | 0.0185 (3) | 0.0228 (3) | −0.0030 (2) | 0.0037 (2) | 0.0032 (2) |
| S2 | 0.0267 (3) | 0.0227 (3) | 0.0238 (3) | 0.0006 (2) | 0.0011 (2) | −0.0032 (2) |
| S3 | 0.0280 (3) | 0.0230 (3) | 0.0299 (3) | 0.0049 (3) | −0.0003 (3) | −0.0037 (3) |
| S4 | 0.0229 (3) | 0.0177 (3) | 0.0279 (3) | −0.0001 (2) | −0.0008 (2) | 0.0003 (2) |
| N1 | 0.0208 (10) | 0.0202 (10) | 0.0198 (10) | −0.0006 (8) | 0.0031 (8) | 0.0034 (8) |
| N2 | 0.0270 (12) | 0.0218 (11) | 0.0267 (11) | 0.0017 (9) | 0.0031 (9) | −0.0053 (9) |
| C1 | 0.0168 (11) | 0.0178 (12) | 0.0212 (12) | 0.0021 (9) | 0.0004 (9) | 0.0021 (10) |
| C2 | 0.0292 (14) | 0.0255 (13) | 0.0203 (13) | −0.0022 (11) | 0.0035 (11) | 0.0061 (10) |
| C3 | 0.0339 (15) | 0.0307 (15) | 0.0231 (13) | −0.0093 (12) | 0.0099 (11) | −0.0019 (11) |
| C4 | 0.0255 (14) | 0.0323 (15) | 0.0362 (15) | −0.0045 (12) | 0.0093 (12) | −0.0052 (12) |
| C5 | 0.0251 (13) | 0.0183 (12) | 0.0236 (13) | −0.0054 (10) | 0.0026 (10) | −0.0003 (10) |
| C6 | 0.0282 (14) | 0.0231 (13) | 0.0218 (13) | −0.0027 (11) | 0.0026 (10) | −0.0005 (10) |
| C7 | 0.0343 (15) | 0.0277 (15) | 0.0315 (15) | 0.0037 (12) | 0.0056 (12) | 0.0024 (12) |
| C8 | 0.0230 (13) | 0.0207 (12) | 0.0198 (12) | 0.0003 (10) | 0.0046 (10) | 0.0007 (10) |
| C9 | 0.0195 (13) | 0.0303 (14) | 0.0299 (14) | 0.0020 (11) | 0.0010 (11) | −0.0008 (12) |
| C10 | 0.0301 (15) | 0.0400 (17) | 0.0379 (17) | 0.0053 (13) | 0.0085 (13) | 0.0092 (13) |
| C11 | 0.052 (2) | 0.057 (2) | 0.0348 (17) | 0.0146 (18) | 0.0035 (15) | 0.0080 (16) |
| C12 | 0.0331 (15) | 0.0317 (15) | 0.0350 (16) | −0.0014 (13) | −0.0007 (12) | −0.0153 (13) |
| C13 | 0.057 (2) | 0.0245 (15) | 0.0402 (17) | −0.0038 (14) | 0.0013 (15) | −0.0074 (13) |
| C14 | 0.055 (2) | 0.042 (2) | 0.080 (3) | −0.0198 (18) | 0.004 (2) | −0.0071 (19) |
| C15 | 0.0203 (12) | 0.0222 (13) | 0.0199 (12) | 0.0026 (10) | 0.0023 (10) | −0.0008 (10) |
| C16 | 0.0245 (13) | 0.0198 (13) | 0.0304 (14) | 0.0001 (11) | 0.0061 (11) | 0.0016 (11) |
| C17 | 0.0225 (13) | 0.0259 (14) | 0.0398 (16) | 0.0013 (11) | 0.0091 (12) | −0.0009 (12) |
| C18 | 0.0282 (14) | 0.0237 (13) | 0.0299 (14) | 0.0080 (11) | 0.0047 (11) | −0.0004 (11) |
| C19 | 0.0348 (15) | 0.0172 (12) | 0.0244 (13) | 0.0003 (11) | 0.0035 (11) | 0.0013 (10) |
| C20 | 0.0223 (12) | 0.0228 (13) | 0.0231 (13) | −0.0025 (10) | 0.0018 (10) | 0.0013 (10) |
| C21 | 0.0212 (12) | 0.0168 (12) | 0.0234 (12) | 0.0043 (10) | 0.0057 (10) | 0.0053 (10) |
| C22 | 0.0278 (14) | 0.0239 (13) | 0.0269 (14) | −0.0019 (11) | 0.0024 (11) | 0.0047 (11) |
| C23 | 0.0414 (17) | 0.0289 (15) | 0.0261 (14) | 0.0008 (13) | 0.0043 (12) | 0.0041 (12) |
| C24 | 0.0372 (16) | 0.0282 (14) | 0.0332 (15) | 0.0069 (12) | 0.0155 (13) | 0.0084 (12) |
| C25 | 0.0284 (14) | 0.0314 (15) | 0.0400 (17) | −0.0041 (12) | 0.0107 (12) | 0.0059 (13) |
| C26 | 0.0227 (13) | 0.0284 (14) | 0.0288 (14) | −0.0011 (11) | 0.0049 (11) | 0.0037 (11) |
| Sn2 | 0.02228 (9) | 0.01617 (9) | 0.01949 (9) | 0.00243 (6) | 0.00069 (6) | −0.00094 (6) |
| S1A | 0.0294 (3) | 0.0214 (3) | 0.0284 (3) | −0.0055 (3) | 0.0061 (3) | −0.0041 (2) |
| S2A | 0.0315 (3) | 0.0225 (3) | 0.0245 (3) | −0.0041 (3) | 0.0036 (3) | −0.0031 (2) |
| S3A | 0.0329 (3) | 0.0218 (3) | 0.0211 (3) | 0.0039 (3) | −0.0005 (3) | −0.0011 (2) |
| S4A | 0.0346 (3) | 0.0196 (3) | 0.0214 (3) | 0.0040 (3) | −0.0007 (3) | −0.0014 (2) |
| N1A | 0.0283 (12) | 0.0245 (12) | 0.0254 (12) | −0.0052 (9) | 0.0021 (9) | −0.0036 (9) |
| N2A | 0.0248 (11) | 0.0191 (11) | 0.0240 (11) | 0.0014 (9) | 0.0024 (9) | −0.0015 (9) |
| C1A | 0.0246 (13) | 0.0213 (13) | 0.0233 (13) | −0.0004 (10) | 0.0012 (10) | 0.0016 (10) |
| C2A | 0.0380 (16) | 0.0343 (16) | 0.0260 (14) | −0.0104 (13) | 0.0057 (12) | −0.0071 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3A | 0.055 (2) | 0.0259 (15) | 0.0326 (16) | −0.0069 (14) | 0.0099 (14) | −0.0063 (12) |
| C4A | 0.051 (2) | 0.0301 (16) | 0.0383 (17) | −0.0024 (14) | 0.0071 (15) | −0.0092 (13) |
| C5A | 0.0270 (14) | 0.0298 (14) | 0.0267 (14) | −0.0035 (12) | 0.0035 (11) | −0.0005 (11) |
| C6A | 0.0364 (17) | 0.0426 (19) | 0.050 (2) | −0.0105 (15) | −0.0057 (15) | 0.0169 (16) |
| C7A | 0.070 (3) | 0.093 (3) | 0.043 (2) | −0.045 (3) | −0.0174 (19) | 0.031 (2) |
| C8A | 0.0227 (12) | 0.0203 (13) | 0.0228 (12) | 0.0001 (10) | 0.0028 (10) | −0.0008 (10) |
| C9A | 0.0285 (14) | 0.0210 (13) | 0.0267 (13) | 0.0034 (11) | 0.0049 (11) | 0.0049 (11) |
| C10A | 0.0296 (14) | 0.0238 (13) | 0.0260 (13) | 0.0057 (11) | 0.0004 (11) | −0.0008 (11) |
| C11A | 0.0273 (14) | 0.0299 (15) | 0.0303 (14) | −0.0005 (12) | 0.0014 (11) | −0.0052 (12) |
| C12A | 0.0277 (14) | 0.0214 (13) | 0.0294 (14) | 0.0026 (11) | 0.0045 (11) | −0.0054 (11) |
| C13A | 0.0337 (15) | 0.0235 (14) | 0.0315 (15) | −0.0045 (12) | −0.0012 (12) | −0.0026 (11) |
| C14A | 0.0269 (14) | 0.0380 (17) | 0.0367 (16) | −0.0042 (13) | −0.0002 (12) | 0.0035 (13) |
| C15A | 0.0177 (12) | 0.0192 (12) | 0.0217 (12) | −0.0005 (10) | 0.0004 (9) | 0.0022 (10) |
| C16A | 0.0266 (13) | 0.0212 (13) | 0.0292 (14) | 0.0026 (11) | 0.0007 (11) | −0.0024 (11) |
| C17A | 0.0232 (13) | 0.0206 (13) | 0.0388 (16) | 0.0042 (11) | 0.0010 (11) | 0.0038 (11) |
| C18A | 0.0203 (13) | 0.0281 (14) | 0.0297 (14) | −0.0021 (11) | −0.0012 (11) | 0.0095 (11) |
| C19A | 0.0257 (13) | 0.0297 (14) | 0.0235 (13) | −0.0017 (11) | 0.0039 (11) | 0.0033 (11) |
| C20A | 0.0204 (12) | 0.0216 (13) | 0.0253 (13) | 0.0019 (10) | 0.0059 (10) | 0.0009 (10) |
| C21A | 0.0221 (12) | 0.0227 (13) | 0.0205 (12) | 0.0006 (10) | 0.0026 (10) | −0.0055 (10) |
| C22A | 0.0244 (13) | 0.0266 (14) | 0.0275 (14) | 0.0021 (11) | 0.0035 (11) | −0.0011 (11) |
| C23A | 0.0318 (15) | 0.0294 (15) | 0.0369 (16) | −0.0001 (12) | 0.0105 (12) | 0.0019 (12) |
| C24A | 0.0273 (14) | 0.0362 (16) | 0.0364 (16) | −0.0063 (12) | 0.0078 (12) | −0.0089 (13) |
| C25A | 0.0226 (14) | 0.0458 (19) | 0.0436 (18) | 0.0012 (13) | −0.0062 (13) | −0.0012 (15) |
| C26A | 0.0282 (15) | 0.0342 (16) | 0.0349 (16) | 0.0012 (12) | −0.0022 (12) | 0.0031 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Sn1—C15 | 2.159 (3) | Sn2—C21A | 2.170 (3) |
| Sn1—C21 | 2.174 (2) | Sn2—C15A | 2.173 (2) |
| Sn1—S1 | 2.5501 (6) | Sn2—S1A | 2.5585 (7) |
| Sn1—S3 | 2.5726 (7) | Sn2—S3A | 2.5700 (6) |
| Sn1—S4 | 2.6754 (6) | Sn2—S4A | 2.6750 (6) |
| Sn1—S2 | 2.7393 (7) | Sn2—S2A | 2.7664 (7) |
| S1—C1 | 1.742 (3) | S1A—C1A | 1.740 (3) |
| S2—C1 | 1.710 (3) | S2A—C1A | 1.704 (3) |
| S3—C8 | 1.738 (3) | S3A—C8A | 1.733 (3) |
| S4—C8 | 1.715 (3) | S4A—C8A | 1.716 (3) |
| N1—C1 | 1.326 (3) | N1A—C1A | 1.328 (4) |
| N1—C2 | 1.465 (3) | N1A—C5A | 1.477 (4) |
| N1—C5 | 1.481 (3) | N1A—C2A | 1.480 (3) |
| N2—C8 | 1.318 (3) | N2A—C8A | 1.327 (3) |
| N2—C12 | 1.477 (3) | N2A—C9A | 1.465 (3) |
| N2—C9 | 1.486 (3) | N2A—C12A | 1.466 (3) |
| C2—C3 | 1.500 (4) | C2A—C3A | 1.496 (5) |
| C2—H2A | 0.9900 | C2A—H2A1 | 0.9900 |
| C2—H2B | 0.9900 | C2A—H2A2 | 0.9900 |
| C3—C4 | 1.317 (4) | C3A—C4A | 1.320 (5) |
| C3—H3 | 0.9500 | C3A—H3A | 0.9500 |

| | | | |
|---|---|---|---|
| C4—H4A | 0.9500 | C4A—H4A1 | 0.9500 |
| C4—H4B | 0.9500 | C4A—H4A2 | 0.9500 |
| C5—C6 | 1.498 (4) | C5A—C6A | 1.484 (4) |
| C5—H5A | 0.9900 | C5A—H5A1 | 0.9900 |
| C5—H5B | 0.9900 | C5A—H5A2 | 0.9900 |
| C6—C7 | 1.314 (4) | C6A—C7A | 1.317 (6) |
| C6—H6 | 0.9500 | C6A—H6A | 0.9500 |
| C7—H7A | 0.9500 | C7A—H7A1 | 0.9500 |
| C7—H7B | 0.9500 | C7A—H7A2 | 0.9500 |
| C9—C10 | 1.496 (4) | C9A—C10A | 1.506 (4) |
| C9—H9A | 0.9900 | C9A—H9A1 | 0.9900 |
| C9—H9B | 0.9900 | C9A—H9A2 | 0.9900 |
| C10—C11 | 1.305 (5) | C10A—C11A | 1.314 (4) |
| C10—H10 | 0.9500 | C10A—H10A | 0.9500 |
| C11—H11A | 0.9500 | C11A—H11C | 0.9500 |
| C11—H11B | 0.9500 | C11A—H11D | 0.9500 |
| C12—C13 | 1.496 (5) | C12A—C13A | 1.501 (4) |
| C12—H12A | 0.9900 | C12A—H12C | 0.9900 |
| C12—H12B | 0.9900 | C12A—H12D | 0.9900 |
| C13—C14 | 1.308 (5) | C13A—C14A | 1.311 (4) |
| C13—H13 | 0.9500 | C13A—H13A | 0.9500 |
| C14—H14A | 0.9500 | C14A—H14C | 0.9500 |
| C14—H14B | 0.9500 | C14A—H14D | 0.9500 |
| C15—C20 | 1.392 (4) | C15A—C16A | 1.393 (4) |
| C15—C16 | 1.396 (4) | C15A—C20A | 1.397 (4) |
| C16—C17 | 1.390 (4) | C16A—C17A | 1.393 (4) |
| C16—H16 | 0.9500 | C16A—H16A | 0.9500 |
| C17—C18 | 1.382 (4) | C17A—C18A | 1.382 (4) |
| C17—H17 | 0.9500 | C17A—H17A | 0.9500 |
| C18—C19 | 1.389 (4) | C18A—C19A | 1.386 (4) |
| C18—H18 | 0.9500 | C18A—H18A | 0.9500 |
| C19—C20 | 1.385 (4) | C19A—C20A | 1.396 (4) |
| C19—H19 | 0.9500 | C19A—H19A | 0.9500 |
| C20—H20 | 0.9500 | C20A—H20A | 0.9500 |
| C21—C26 | 1.391 (4) | C21A—C22A | 1.386 (4) |
| C21—C22 | 1.393 (4) | C21A—C26A | 1.395 (4) |
| C22—C23 | 1.387 (4) | C22A—C23A | 1.400 (4) |
| C22—H22 | 0.9500 | C22A—H22A | 0.9500 |
| C23—C24 | 1.382 (4) | C23A—C24A | 1.380 (4) |
| C23—H23 | 0.9500 | C23A—H23A | 0.9500 |
| C24—C25 | 1.384 (4) | C24A—C25A | 1.373 (5) |
| C24—H24 | 0.9500 | C24A—H24A | 0.9500 |
| C25—C26 | 1.394 (4) | C25A—C26A | 1.396 (4) |
| C25—H25 | 0.9500 | C25A—H25A | 0.9500 |
| C26—H26 | 0.9500 | C26A—H26A | 0.9500 |
| | | | |
| C15—Sn1—C21 | 99.84 (9) | C21A—Sn2—C15A | 103.34 (9) |
| C15—Sn1—S1 | 104.01 (7) | C21A—Sn2—S1A | 96.36 (7) |

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|---|---|---|---|
| C21—Sn1—S1 | 92.77 (7) | C15A—Sn2—S1A | 101.31 (7) |
| C15—Sn1—S3 | 94.80 (7) | C21A—Sn2—S3A | 105.20 (7) |
| C21—Sn1—S3 | 101.09 (7) | C15A—Sn2—S3A | 95.16 (7) |
| S1—Sn1—S3 | 154.38 (2) | S1A—Sn2—S3A | 149.00 (2) |
| C15—Sn1—S4 | 160.59 (7) | C21A—Sn2—S4A | 92.74 (7) |
| C21—Sn1—S4 | 92.52 (7) | C15A—Sn2—S4A | 159.91 (7) |
| S1—Sn1—S4 | 90.18 (2) | S1A—Sn2—S4A | 88.58 (2) |
| S3—Sn1—S4 | 67.97 (2) | S3A—Sn2—S4A | 68.69 (2) |
| C15—Sn1—S2 | 91.81 (7) | C21A—Sn2—S2A | 161.40 (7) |
| C21—Sn1—S2 | 159.42 (7) | C15A—Sn2—S2A | 88.92 (7) |
| S1—Sn1—S2 | 67.824 (19) | S1A—Sn2—S2A | 67.18 (2) |
| S3—Sn1—S2 | 94.71 (2) | S3A—Sn2—S2A | 87.26 (2) |
| S4—Sn1—S2 | 81.21 (2) | S4A—Sn2—S2A | 78.76 (2) |
| C1—S1—Sn1 | 89.92 (8) | C1A—S1A—Sn2 | 90.15 (9) |
| C1—S2—Sn1 | 84.47 (9) | C1A—S2A—Sn2 | 84.16 (9) |
| C8—S3—Sn1 | 89.22 (9) | C8A—S3A—Sn2 | 87.98 (9) |
| C8—S4—Sn1 | 86.37 (9) | C8A—S4A—Sn2 | 84.96 (9) |
| C1—N1—C2 | 122.5 (2) | C1A—N1A—C5A | 122.0 (2) |
| C1—N1—C5 | 122.6 (2) | C1A—N1A—C2A | 123.4 (2) |
| C2—N1—C5 | 114.9 (2) | C5A—N1A—C2A | 114.5 (2) |
| C8—N2—C12 | 122.5 (2) | C8A—N2A—C9A | 122.4 (2) |
| C8—N2—C9 | 122.6 (2) | C8A—N2A—C12A | 122.1 (2) |
| C12—N2—C9 | 114.8 (2) | C9A—N2A—C12A | 115.5 (2) |
| N1—C1—S2 | 123.62 (19) | N1A—C1A—S2A | 122.7 (2) |
| N1—C1—S1 | 118.58 (19) | N1A—C1A—S1A | 119.4 (2) |
| S2—C1—S1 | 117.77 (14) | S2A—C1A—S1A | 117.94 (16) |
| N1—C2—C3 | 112.5 (2) | N1A—C2A—C3A | 110.9 (2) |
| N1—C2—H2A | 109.1 | N1A—C2A—H2A1 | 109.5 |
| C3—C2—H2A | 109.1 | C3A—C2A—H2A1 | 109.5 |
| N1—C2—H2B | 109.1 | N1A—C2A—H2A2 | 109.5 |
| C3—C2—H2B | 109.1 | C3A—C2A—H2A2 | 109.5 |
| H2A—C2—H2B | 107.8 | H2A1—C2A—H2A2 | 108.1 |
| C4—C3—C2 | 126.2 (3) | C4A—C3A—C2A | 123.2 (3) |
| C4—C3—H3 | 116.9 | C4A—C3A—H3A | 118.4 |
| C2—C3—H3 | 116.9 | C2A—C3A—H3A | 118.4 |
| C3—C4—H4A | 120.0 | C3A—C4A—H4A1 | 120.0 |
| C3—C4—H4B | 120.0 | C3A—C4A—H4A2 | 120.0 |
| H4A—C4—H4B | 120.0 | H4A1—C4A—H4A2 | 120.0 |
| N1—C5—C6 | 111.3 (2) | N1A—C5A—C6A | 110.9 (2) |
| N1—C5—H5A | 109.4 | N1A—C5A—H5A1 | 109.5 |
| C6—C5—H5A | 109.4 | C6A—C5A—H5A1 | 109.5 |
| N1—C5—H5B | 109.4 | N1A—C5A—H5A2 | 109.5 |
| C6—C5—H5B | 109.4 | C6A—C5A—H5A2 | 109.5 |
| H5A—C5—H5B | 108.0 | H5A1—C5A—H5A2 | 108.0 |
| C7—C6—C5 | 124.0 (3) | C7A—C6A—C5A | 122.9 (4) |
| C7—C6—H6 | 118.0 | C7A—C6A—H6A | 118.5 |
| C5—C6—H6 | 118.0 | C5A—C6A—H6A | 118.5 |
| C6—C7—H7A | 120.0 | C6A—C7A—H7A1 | 120.0 |

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|---|---|---|---|
| C6—C7—H7B | 120.0 | C6A—C7A—H7A2 | 120.0 |
| H7A—C7—H7B | 120.0 | H7A1—C7A—H7A2 | 120.0 |
| N2—C8—S4 | 122.3 (2) | N2A—C8A—S4A | 121.67 (19) |
| N2—C8—S3 | 121.3 (2) | N2A—C8A—S3A | 120.11 (19) |
| S4—C8—S3 | 116.40 (15) | S4A—C8A—S3A | 118.21 (15) |
| N2—C9—C10 | 109.6 (2) | N2A—C9A—C10A | 113.2 (2) |
| N2—C9—H9A | 109.8 | N2A—C9A—H9A1 | 108.9 |
| C10—C9—H9A | 109.8 | C10A—C9A—H9A1 | 108.9 |
| N2—C9—H9B | 109.8 | N2A—C9A—H9A2 | 108.9 |
| C10—C9—H9B | 109.8 | C10A—C9A—H9A2 | 108.9 |
| H9A—C9—H9B | 108.2 | H9A1—C9A—H9A2 | 107.7 |
| C11—C10—C9 | 123.4 (3) | C11A—C10A—C9A | 126.1 (3) |
| C11—C10—H10 | 118.3 | C11A—C10A—H10A | 117.0 |
| C9—C10—H10 | 118.3 | C9A—C10A—H10A | 117.0 |
| C10—C11—H11A | 120.0 | C10A—C11A—H11C | 120.0 |
| C10—C11—H11B | 120.0 | C10A—C11A—H11D | 120.0 |
| H11A—C11—H11B | 120.0 | H11C—C11A—H11D | 120.0 |
| N2—C12—C13 | 110.8 (2) | N2A—C12A—C13A | 112.3 (2) |
| N2—C12—H12A | 109.5 | N2A—C12A—H12C | 109.1 |
| C13—C12—H12A | 109.5 | C13A—C12A—H12C | 109.1 |
| N2—C12—H12B | 109.5 | N2A—C12A—H12D | 109.1 |
| C13—C12—H12B | 109.5 | C13A—C12A—H12D | 109.1 |
| H12A—C12—H12B | 108.1 | H12C—C12A—H12D | 107.9 |
| C14—C13—C12 | 123.8 (3) | C14A—C13A—C12A | 126.5 (3) |
| C14—C13—H13 | 118.1 | C14A—C13A—H13A | 116.7 |
| C12—C13—H13 | 118.1 | C12A—C13A—H13A | 116.7 |
| C13—C14—H14A | 120.0 | C13A—C14A—H14C | 120.0 |
| C13—C14—H14B | 120.0 | C13A—C14A—H14D | 120.0 |
| H14A—C14—H14B | 120.0 | H14C—C14A—H14D | 120.0 |
| C20—C15—C16 | 118.6 (2) | C16A—C15A—C20A | 118.3 (2) |
| C20—C15—Sn1 | 118.07 (19) | C16A—C15A—Sn2 | 120.81 (19) |
| C16—C15—Sn1 | 123.31 (19) | C20A—C15A—Sn2 | 120.91 (18) |
| C17—C16—C15 | 120.3 (2) | C17A—C16A—C15A | 121.1 (3) |
| C17—C16—H16 | 119.8 | C17A—C16A—H16A | 119.5 |
| C15—C16—H16 | 119.8 | C15A—C16A—H16A | 119.5 |
| C18—C17—C16 | 120.4 (3) | C18A—C17A—C16A | 119.8 (3) |
| C18—C17—H17 | 119.8 | C18A—C17A—H17A | 120.1 |
| C16—C17—H17 | 119.8 | C16A—C17A—H17A | 120.1 |
| C19—C18—C17 | 119.9 (3) | C17A—C18A—C19A | 120.3 (2) |
| C19—C18—H18 | 120.1 | C17A—C18A—H18A | 119.9 |
| C17—C18—H18 | 120.1 | C19A—C18A—H18A | 119.9 |
| C18—C19—C20 | 119.7 (2) | C18A—C19A—C20A | 119.7 (3) |
| C18—C19—H19 | 120.2 | C18A—C19A—H19A | 120.2 |
| C20—C19—H19 | 120.2 | C20A—C19A—H19A | 120.2 |
| C19—C20—C15 | 121.2 (2) | C15A—C20A—C19A | 120.9 (2) |
| C19—C20—H20 | 119.4 | C15A—C20A—H20A | 119.6 |
| C15—C20—H20 | 119.4 | C19A—C20A—H20A | 119.6 |
| C26—C21—C22 | 117.6 (2) | C22A—C21A—C26A | 118.0 (3) |

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|---|---|---|---|
| C26—C21—Sn1 | 123.63 (19) | C22A—C21A—Sn2 | 118.00 (19) |
| C22—C21—Sn1 | 118.80 (19) | C26A—C21A—Sn2 | 124.0 (2) |
| C23—C22—C21 | 121.4 (3) | C21A—C22A—C23A | 121.3 (3) |
| C23—C22—H22 | 119.3 | C21A—C22A—H22A | 119.4 |
| C21—C22—H22 | 119.3 | C23A—C22A—H22A | 119.4 |
| C24—C23—C22 | 120.2 (3) | C24A—C23A—C22A | 119.7 (3) |
| C24—C23—H23 | 119.9 | C24A—C23A—H23A | 120.1 |
| C22—C23—H23 | 119.9 | C22A—C23A—H23A | 120.1 |
| C23—C24—C25 | 119.4 (3) | C25A—C24A—C23A | 119.7 (3) |
| C23—C24—H24 | 120.3 | C25A—C24A—H24A | 120.1 |
| C25—C24—H24 | 120.3 | C23A—C24A—H24A | 120.1 |
| C24—C25—C26 | 120.1 (3) | C24A—C25A—C26A | 120.7 (3) |
| C24—C25—H25 | 120.0 | C24A—C25A—H25A | 119.7 |
| C26—C25—H25 | 120.0 | C26A—C25A—H25A | 119.7 |
| C21—C26—C25 | 121.3 (3) | C21A—C26A—C25A | 120.5 (3) |
| C21—C26—H26 | 119.4 | C21A—C26A—H26A | 119.8 |
| C25—C26—H26 | 119.4 | C25A—C26A—H26A | 119.8 |
| | | | |
| C2—N1—C1—S2 | 0.1 (3) | C5A—N1A—C1A—S2A | 4.7 (4) |
| C5—N1—C1—S2 | 179.23 (18) | C2A—N1A—C1A—S2A | −175.2 (2) |
| C2—N1—C1—S1 | −178.18 (18) | C5A—N1A—C1A—S1A | −175.4 (2) |
| C5—N1—C1—S1 | 1.0 (3) | C2A—N1A—C1A—S1A | 4.8 (4) |
| Sn1—S2—C1—N1 | −177.4 (2) | Sn2—S2A—C1A—N1A | 172.9 (2) |
| Sn1—S2—C1—S1 | 0.89 (13) | Sn2—S2A—C1A—S1A | −7.00 (14) |
| Sn1—S1—C1—N1 | 177.43 (19) | Sn2—S1A—C1A—N1A | −172.4 (2) |
| Sn1—S1—C1—S2 | −0.95 (13) | Sn2—S1A—C1A—S2A | 7.53 (15) |
| C1—N1—C2—C3 | −95.8 (3) | C1A—N1A—C2A—C3A | −98.2 (3) |
| C5—N1—C2—C3 | 85.0 (3) | C5A—N1A—C2A—C3A | 81.9 (3) |
| N1—C2—C3—C4 | 12.5 (4) | N1A—C2A—C3A—C4A | −105.2 (3) |
| C1—N1—C5—C6 | −91.2 (3) | C1A—N1A—C5A—C6A | −97.9 (3) |
| C2—N1—C5—C6 | 88.0 (3) | C2A—N1A—C5A—C6A | 82.0 (3) |
| N1—C5—C6—C7 | −122.3 (3) | N1A—C5A—C6A—C7A | −114.6 (4) |
| C12—N2—C8—S4 | 179.3 (2) | C9A—N2A—C8A—S4A | 2.4 (4) |
| C9—N2—C8—S4 | 1.2 (4) | C12A—N2A—C8A—S4A | −173.87 (19) |
| C12—N2—C8—S3 | −0.7 (4) | C9A—N2A—C8A—S3A | −178.66 (19) |
| C9—N2—C8—S3 | −178.79 (19) | C12A—N2A—C8A—S3A | 5.1 (3) |
| Sn1—S4—C8—N2 | 178.1 (2) | Sn2—S4A—C8A—N2A | 175.2 (2) |
| Sn1—S4—C8—S3 | −1.92 (13) | Sn2—S4A—C8A—S3A | −3.74 (14) |
| Sn1—S3—C8—N2 | −178.1 (2) | Sn2—S3A—C8A—N2A | −175.1 (2) |
| Sn1—S3—C8—S4 | 1.99 (14) | Sn2—S3A—C8A—S4A | 3.88 (15) |
| C8—N2—C9—C10 | 101.8 (3) | C8A—N2A—C9A—C10A | 88.1 (3) |
| C12—N2—C9—C10 | −76.4 (3) | C12A—N2A—C9A—C10A | −95.3 (3) |
| N2—C9—C10—C11 | 105.3 (3) | N2A—C9A—C10A—C11A | −9.9 (4) |
| C8—N2—C12—C13 | 104.1 (3) | C8A—N2A—C12A—C13A | 90.9 (3) |
| C9—N2—C12—C13 | −77.6 (3) | C9A—N2A—C12A—C13A | −85.6 (3) |
| N2—C12—C13—C14 | 110.9 (4) | N2A—C12A—C13A—C14A | −13.3 (4) |
| C20—C15—C16—C17 | −0.4 (4) | C20A—C15A—C16A—C17A | 0.9 (4) |
| Sn1—C15—C16—C17 | 176.7 (2) | Sn2—C15A—C16A—C17A | −177.9 (2) |

| | | | |
|---|---|---|---|
| C15—C16—C17—C18 | 0.9 (4) | C15A—C16A—C17A—C18A | −0.7 (4) |
| C16—C17—C18—C19 | −0.7 (4) | C16A—C17A—C18A—C19A | −0.1 (4) |
| C17—C18—C19—C20 | 0.0 (4) | C17A—C18A—C19A—C20A | 0.7 (4) |
| C18—C19—C20—C15 | 0.6 (4) | C16A—C15A—C20A—C19A | −0.3 (4) |
| C16—C15—C20—C19 | −0.4 (4) | Sn2—C15A—C20A—C19A | 178.47 (19) |
| Sn1—C15—C20—C19 | −177.60 (19) | C18A—C19A—C20A—C15A | −0.5 (4) |
| C26—C21—C22—C23 | −0.7 (4) | C26A—C21A—C22A—C23A | −1.2 (4) |
| Sn1—C21—C22—C23 | 180.0 (2) | Sn2—C21A—C22A—C23A | 179.5 (2) |
| C21—C22—C23—C24 | −0.2 (4) | C21A—C22A—C23A—C24A | 1.1 (4) |
| C22—C23—C24—C25 | 0.5 (4) | C22A—C23A—C24A—C25A | −0.4 (4) |
| C23—C24—C25—C26 | 0.1 (4) | C23A—C24A—C25A—C26A | −0.1 (5) |
| C22—C21—C26—C25 | 1.2 (4) | C22A—C21A—C26A—C25A | 0.7 (4) |
| Sn1—C21—C26—C25 | −179.5 (2) | Sn2—C21A—C26A—C25A | 180.0 (2) |
| C24—C25—C26—C21 | −0.9 (4) | C24A—C25A—C26A—C21A | −0.1 (5) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 and *Cg*2 are the centroids of the (C15*A*–C20*A*) and (C21*A*–C26*A*) rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7*A*···*Cg*1$^{i}$ | 0.95 | 2.83 | 3.774 (3) | 172 |
| C7—H7*B*···*Cg*2$^{ii}$ | 0.95 | 2.92 | 3.582 (3) | 128 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.