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## Structure Reports

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**(N-Benzyl-N-ethyldithiocarbamato)-di-tert-butylchloridotin(IV)**Amirah Faizah Abdul Muthalib,<sup>a</sup> Ibrahim Baba,<sup>a‡</sup>  
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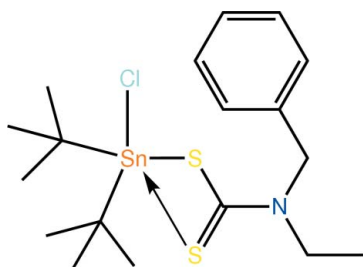
Received 16 February 2011; accepted 20 February 2011

Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.018;  $wR$  factor = 0.046; data-to-parameter ratio = 22.6.

The Sn<sup>IV</sup> atom in the title diorganotin dithiocarbamate, [Sn(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>Cl(C<sub>10</sub>H<sub>12</sub>NS<sub>2</sub>)], is pentacoordinated by an asymmetrically coordinating dithiocarbamate ligand, a Cl and two C atoms of the Sn-bound *tert*-butyl groups. The resulting C<sub>2</sub>ClS<sub>2</sub> donor set defines a coordination geometry intermediate between square pyramidal and trigonal bipyramidal with a slight tendency towards the former. In the crystal structure, C—H... $\pi$  contacts link centrosymmetrically related molecules into dimeric aggregates.

## Related literature

For a review on the applications and structural chemistry of tin dithiocarbamates, see: Tiekink (2008). For additional structural analysis, see: Addison *et al.* (1984); Spek (2009). For a recently reported related structure, see: Abdul Muthalib *et al.* (2010).



## Experimental

## Crystal data

[Sn(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>Cl(C<sub>10</sub>H<sub>12</sub>NS<sub>2</sub>)] $M_r = 478.69$ <sup>‡</sup> Additional correspondence author, e-mail: aibi@ukm.my.Triclinic,  $P\bar{1}$   
 $a = 8.6140$  (2) Å  
 $b = 10.9604$  (3) Å  
 $c = 11.4765$  (3) Å  
 $\alpha = 91.858$  (2)°  
 $\beta = 96.193$  (2)°  
 $\gamma = 96.011$  (2)° $V = 1070.24$  (5) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 1.51$  mm<sup>-1</sup>  
 $T = 150$  K  
 $0.30 \times 0.23 \times 0.16$  mm

## Data collection

Oxford Diffraction Xcaliber Eos  
Gemini diffractometer  
Absorption correction: multi-scan  
(*CrysAlis PRO*; Oxford  
Diffraction, 2010)  
 $T_{\min} = 0.935$ ,  $T_{\max} = 1.000$ 26998 measured reflections  
4865 independent reflections  
4707 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.018$   
 $wR(F^2) = 0.046$   
 $S = 1.11$   
4865 reflections215 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.50$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

|        |            |        |             |
|--------|------------|--------|-------------|
| Sn—Cl1 | 2.4847 (4) | Sn—C11 | 2.1884 (14) |
| Sn—S1  | 2.4760 (4) | Sn—C15 | 2.1879 (15) |
| Sn—S2  | 2.7409 (4) |        |             |

Table 2

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C5–C10 ring.

| $D-H\cdots A$               | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------|-------|-------------|-------------|---------------|
| C3—H3a...Cg1                | 0.98  | 2.78        | 3.6491 (18) | 149           |
| C13—H13b...Cg1 <sup>i</sup> | 0.98  | 2.96        | 3.5401 (18) | 119           |

Symmetry code: (i)  $-x + 1, -y, -z + 1$ .

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2099).

## References

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## supporting information

*Acta Cryst.* (2011). E67, m372–m373 [doi:10.1107/S1600536811006398]

**(*N*-Benzyl-*N*-ethyldithiocarbamato)di-*tert*-butylchloridotin(IV)**

**Amirah Faizah Abdul Muthalib, Ibrahim Baba, Mohamed Ibrahim Mohamed Tahir and Edward R. T. Tiekink**

**S1. Comment**

Organotin dithiocarbamates attract attention as they exhibit properties suggesting their potential as anti-cancer agents, anti-microbials and insecticides (Tiekink, 2008). Motivated by these and in continuation of structural studies of these systems (Abdul Muthalib *et al.*, 2010), the analysis of the title compound, (I), was undertaken.

The Sn<sup>IV</sup> atom in (I) is five-coordinated, being chelated by an asymmetrically coordinating dithiocarbamate ligand, a Cl and two C atoms of the Sn-bound *tert*-butyl groups (Fig. 1 and Table 1). The asymmetric chelating mode of the non-symmetric dithiocarbamate ligand is reflected in the non-equivalence of the associated C $\cdots$ S bond distances (Table 1). The coordination geometry is intermediate between square pyramidal and trigonal bi-pyramidal with a leaning towards the former. This assignment is based on the value calculated for  $\tau$  of 0.45 for the Sn atom, which compares to the  $\tau$  values of 0.0 and 1.0 for ideal square pyramidal and trigonal bi-pyramidal geometries, respectively (Spek, 2009; Addison *et al.*, 1984). The mode of coordination of the dithiocarbamate ligand, the disposition of the ligand donor set, and the intermediate coordination geometry observed for (I) matches with the literature precedents (Tiekink, 2008).

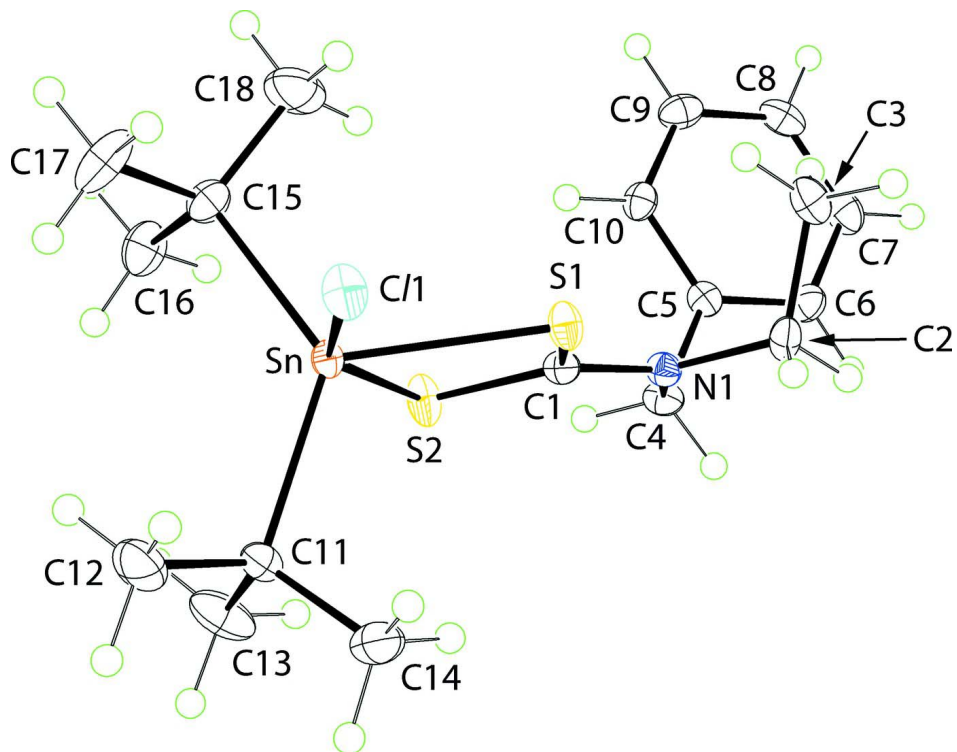
The most prominent feature of the crystal packing is the presence of C–H $\cdots$  $\pi$  interactions (Table 2). As shown in Fig. 2, these lead to dimeric aggregates. It is also noted that intramolecular C–H $\cdots$  $\pi$  contacts are present so that the benzene ring participates in two such interactions (Table 2, Fig. 2). The dimeric aggregates stack into columns along the *a* axis (Fig. 3).

**S2. Experimental**

The dithiocarbamate ligand was prepared by the addition of carbon disulfide (0.01 mol) to an ethanolic solution (20 ml) of ethylbenzylamine (0.01 mol). The mixture was stirred for 1 h at 277 K, after which the solution was added drop wise to a solution of di-*tert*-butyltin(IV) dichloride (0.005 mol) in ethanol (20 ml). The resulting mixture was stirred for 1 h. The white precipitate was filtered, washed with cold ethanol and dried in a desiccator. Crystallization was carried out by using an ethanol:chloroform (1:2) mixture. Yield 76%; m.p. 451–453 K. Elemental analysis. Found (calculated) for C<sub>18</sub>H<sub>30</sub>ClNS<sub>2</sub>Sn: C, 44.81 (45.16); H 6.27 (6.32), N 2.72 (2.93), S 13.23 (13.40); Sn 23.98 (24.80) %. UV (CHCl<sub>3</sub>)  $\lambda_{\max}$  244 (*L*( $\pi$ )  $\rightarrow$  *L*( $\pi^*$ )). IR (KBr):  $\nu$ (C–H) 2933*m*, 2958*m*;  $\nu$ (C $\cdots$ N) 1496*m*;  $\nu$ (N–C) 1185 s;  $\nu$ (C $\cdots$ S) 950 s;  $\nu$ (Sn–S) 351 s cm<sup>-1</sup>.

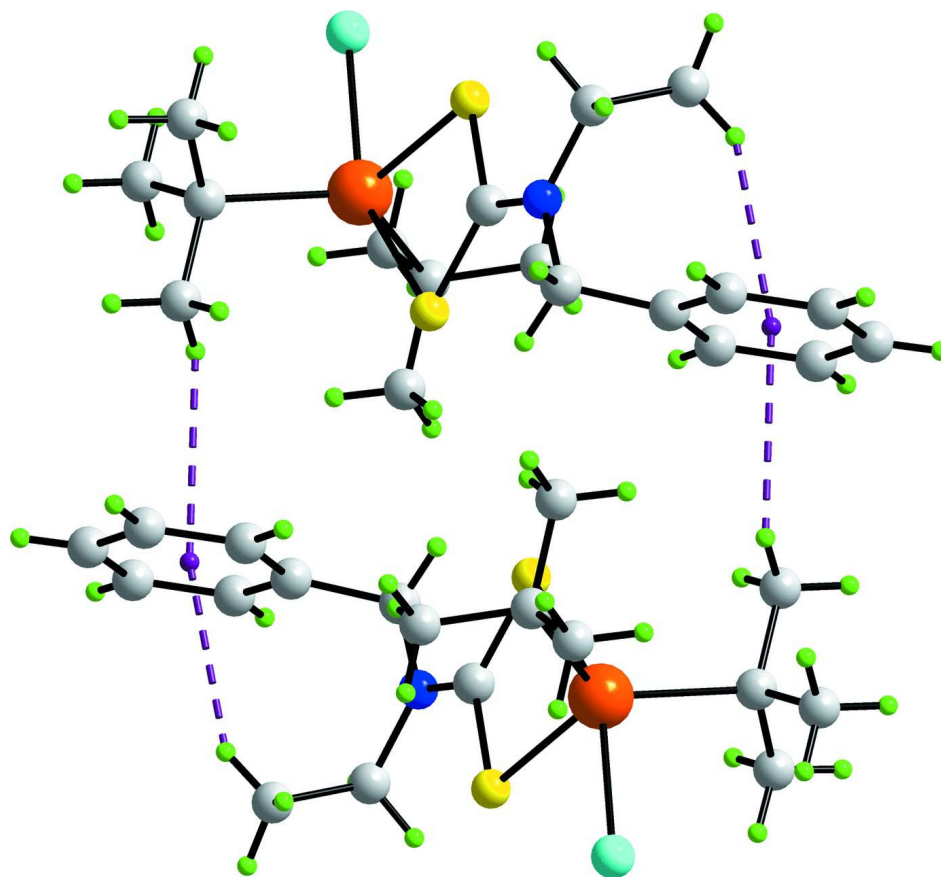
**S3. Refinement**

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



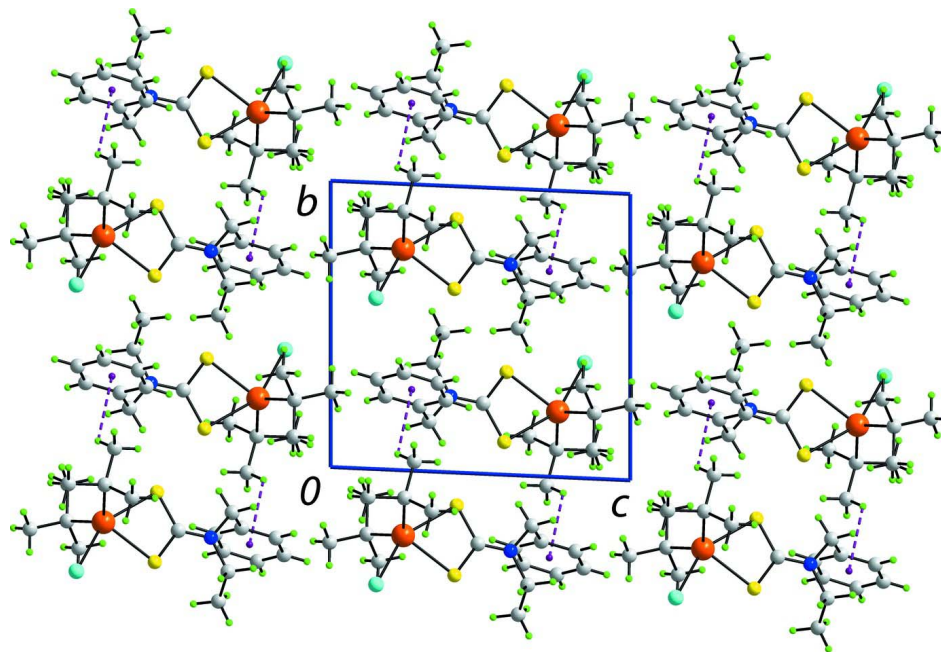
**Figure 1**

The molecular structure of of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.



**Figure 2**

A view of the dimeric aggregate in (I) showing the intra- and intermolecular C–H... $\pi$  contacts as purple dashed lines.

**Figure 3**

A view in projection down the  $a$  axis of (I) showing columns of dimeric aggregates along  $a$ . The intermolecular C–H $\cdots$  $\pi$  contacts are shown as purple dashed lines.

**(*N*-Benzyl-*N*-ethylthiocarbamato)di-*tert*-butylchloridotin(IV)**

*Crystal data*

[Sn(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>Cl(C<sub>10</sub>H<sub>12</sub>NS<sub>2</sub>)]

$M_r = 478.69$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 8.6140$  (2) Å

$b = 10.9604$  (3) Å

$c = 11.4765$  (3) Å

$\alpha = 91.858$  (2)°

$\beta = 96.193$  (2)°

$\gamma = 96.011$  (2)°

$V = 1070.24$  (5) Å<sup>3</sup>

$Z = 2$

$F(000) = 488$

$D_x = 1.485$  Mg m<sup>-3</sup>

Melting point = 451–453 K

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

Cell parameters from 22888 reflections

$\theta = 2.4$ – $28.8$ °

$\mu = 1.51$  mm<sup>-1</sup>

$T = 150$  K

Block, colourless

$0.30 \times 0.23 \times 0.16$  mm

*Data collection*

Oxford Diffraction Xcaliber Eos Gemini diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.1952 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2010)

$T_{\min} = 0.935$ ,  $T_{\max} = 1.000$

26998 measured reflections

4865 independent reflections

4707 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 2.4$ °

$h = -11 \rightarrow 11$

$k = -13 \rightarrow 13$

$l = -14 \rightarrow 14$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.018$   
 $wR(F^2) = 0.046$   
 $S = 1.11$   
 4865 reflections  
 215 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 0.279P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.003$   
 $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$

Special details

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

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

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

|     | $x$           | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| Sn  | 0.908142 (10) | 0.227855 (8) | 0.757926 (8) | 0.01355 (4)                      |
| Cl1 | 1.09329 (4)   | 0.40294 (3)  | 0.84821 (3)  | 0.02158 (8)                      |
| S1  | 0.88193 (4)   | 0.35904 (3)  | 0.58681 (3)  | 0.01801 (8)                      |
| S2  | 0.70139 (5)   | 0.11432 (3)  | 0.57914 (3)  | 0.02180 (8)                      |
| N1  | 0.69363 (14)  | 0.26534 (11) | 0.39968 (10) | 0.0152 (2)                       |
| C1  | 0.74996 (17)  | 0.24573 (13) | 0.50861 (12) | 0.0154 (3)                       |
| C2  | 0.73841 (18)  | 0.38150 (14) | 0.34275 (13) | 0.0192 (3)                       |
| H2A | 0.7233        | 0.3660       | 0.2566       | 0.023*                           |
| H2B | 0.8514        | 0.4073       | 0.3659       | 0.023*                           |
| C3  | 0.6448 (2)    | 0.48595 (15) | 0.37411 (15) | 0.0248 (3)                       |
| H3A | 0.5338        | 0.4643       | 0.3450       | 0.037*                           |
| H3B | 0.6849        | 0.5609       | 0.3380       | 0.037*                           |
| H3C | 0.6555        | 0.4998       | 0.4595       | 0.037*                           |
| C4  | 0.58006 (18)  | 0.17438 (14) | 0.32856 (13) | 0.0185 (3)                       |
| H4A | 0.5613        | 0.0996       | 0.3734       | 0.022*                           |
| H4B | 0.6243        | 0.1508       | 0.2560       | 0.022*                           |
| C5  | 0.42662 (17)  | 0.22668 (13) | 0.29687 (13) | 0.0162 (3)                       |
| C6  | 0.38063 (18)  | 0.25643 (15) | 0.18239 (13) | 0.0206 (3)                       |
| H6  | 0.4422        | 0.2374       | 0.1217       | 0.025*                           |
| C7  | 0.24535 (19)  | 0.31377 (15) | 0.15584 (14) | 0.0248 (3)                       |
| H7  | 0.2146        | 0.3341       | 0.0775       | 0.030*                           |
| C8  | 0.15570 (19)  | 0.34106 (14) | 0.24459 (15) | 0.0244 (3)                       |
| H8  | 0.0644        | 0.3818       | 0.2273       | 0.029*                           |
| C9  | 0.19895 (18)  | 0.30901 (15) | 0.35845 (15) | 0.0230 (3)                       |
| H9  | 0.1362        | 0.3265       | 0.4188       | 0.028*                           |

|      |              |               |              |            |
|------|--------------|---------------|--------------|------------|
| C10  | 0.33337 (17) | 0.25166 (14)  | 0.38442 (13) | 0.0185 (3) |
| H10  | 0.3621       | 0.2293        | 0.4624       | 0.022*     |
| C11  | 1.08251 (17) | 0.09669 (13)  | 0.75357 (13) | 0.0182 (3) |
| C12  | 1.1743 (2)   | 0.09891 (18)  | 0.87481 (16) | 0.0344 (4) |
| H12A | 1.2538       | 0.0413        | 0.8745       | 0.052*     |
| H12B | 1.1022       | 0.0749        | 0.9326       | 0.052*     |
| H12C | 1.2258       | 0.1820        | 0.8954       | 0.052*     |
| C13  | 1.0023 (2)   | -0.03233 (15) | 0.7207 (2)   | 0.0351 (4) |
| H13A | 0.9457       | -0.0337       | 0.6418       | 0.053*     |
| H13B | 0.9280       | -0.0558       | 0.7771       | 0.053*     |
| H13C | 1.0816       | -0.0903       | 0.7221       | 0.053*     |
| C14  | 1.1918 (2)   | 0.13760 (17)  | 0.66298 (17) | 0.0334 (4) |
| H14A | 1.2413       | 0.2211        | 0.6843       | 0.050*     |
| H14B | 1.1312       | 0.1364        | 0.5855       | 0.050*     |
| H14C | 1.2731       | 0.0816        | 0.6609       | 0.050*     |
| C15  | 0.72963 (18) | 0.22899 (15)  | 0.87978 (13) | 0.0210 (3) |
| C16  | 0.6414 (2)   | 0.10044 (16)  | 0.87739 (15) | 0.0283 (4) |
| H16A | 0.5648       | 0.0983        | 0.9347       | 0.042*     |
| H16B | 0.7162       | 0.0408        | 0.8971       | 0.042*     |
| H16C | 0.5866       | 0.0797        | 0.7988       | 0.042*     |
| C17  | 0.8116 (2)   | 0.2629 (2)    | 1.00325 (15) | 0.0356 (4) |
| H17A | 0.8685       | 0.3453        | 1.0046       | 0.053*     |
| H17B | 0.8857       | 0.2034        | 1.0253       | 0.053*     |
| H17C | 0.7330       | 0.2618        | 1.0590       | 0.053*     |
| C18  | 0.6177 (2)   | 0.32236 (19)  | 0.8403 (2)   | 0.0390 (5) |
| H18A | 0.5717       | 0.3013        | 0.7594       | 0.059*     |
| H18B | 0.6756       | 0.4045        | 0.8444       | 0.059*     |
| H18C | 0.5339       | 0.3212        | 0.8918       | 0.059*     |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$      | $U^{23}$     |
|-----|--------------|--------------|--------------|---------------|---------------|--------------|
| Sn  | 0.01353 (6)  | 0.01384 (6)  | 0.01283 (6)  | 0.00071 (4)   | -0.00031 (4)  | 0.00204 (4)  |
| Cl1 | 0.02389 (18) | 0.01842 (18) | 0.01980 (17) | -0.00371 (14) | -0.00377 (14) | 0.00095 (13) |
| S1  | 0.02071 (18) | 0.01593 (17) | 0.01529 (16) | -0.00302 (13) | -0.00340 (13) | 0.00330 (13) |
| S2  | 0.0271 (2)   | 0.01675 (18) | 0.01827 (17) | -0.00533 (15) | -0.00567 (15) | 0.00382 (14) |
| N1  | 0.0147 (6)   | 0.0160 (6)   | 0.0144 (6)   | 0.0026 (5)    | -0.0006 (5)   | 0.0002 (5)   |
| C1  | 0.0146 (6)   | 0.0164 (7)   | 0.0150 (6)   | 0.0026 (5)    | 0.0005 (5)    | -0.0010 (5)  |
| C2  | 0.0198 (7)   | 0.0232 (8)   | 0.0148 (7)   | 0.0010 (6)    | 0.0023 (6)    | 0.0058 (6)   |
| C3  | 0.0268 (8)   | 0.0179 (8)   | 0.0292 (8)   | 0.0013 (6)    | 0.0012 (7)    | 0.0057 (6)   |
| C4  | 0.0196 (7)   | 0.0188 (7)   | 0.0160 (7)   | 0.0042 (6)    | -0.0031 (6)   | -0.0051 (5)  |
| C5  | 0.0170 (7)   | 0.0143 (7)   | 0.0160 (7)   | -0.0001 (5)   | -0.0019 (5)   | -0.0014 (5)  |
| C6  | 0.0218 (7)   | 0.0247 (8)   | 0.0152 (7)   | 0.0028 (6)    | 0.0007 (6)    | -0.0009 (6)  |
| C7  | 0.0262 (8)   | 0.0254 (8)   | 0.0210 (8)   | 0.0038 (6)    | -0.0069 (6)   | 0.0033 (6)   |
| C8  | 0.0190 (7)   | 0.0183 (8)   | 0.0351 (9)   | 0.0048 (6)    | -0.0032 (7)   | -0.0005 (7)  |
| C9  | 0.0199 (7)   | 0.0220 (8)   | 0.0267 (8)   | -0.0005 (6)   | 0.0054 (6)    | -0.0057 (6)  |
| C10 | 0.0198 (7)   | 0.0197 (7)   | 0.0151 (7)   | -0.0009 (6)   | 0.0008 (6)    | -0.0003 (5)  |
| C11 | 0.0173 (7)   | 0.0152 (7)   | 0.0225 (7)   | 0.0034 (5)    | 0.0018 (6)    | 0.0023 (6)   |



|     |             |             |             |             |             |             |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C12 | 0.0352 (10) | 0.0406 (11) | 0.0287 (9)  | 0.0197 (8)  | -0.0058 (8) | 0.0024 (8)  |
| C13 | 0.0275 (9)  | 0.0155 (8)  | 0.0613 (13) | 0.0039 (7)  | -0.0013 (9) | 0.0013 (8)  |
| C14 | 0.0362 (10) | 0.0296 (10) | 0.0402 (10) | 0.0125 (8)  | 0.0202 (8)  | 0.0069 (8)  |
| C15 | 0.0190 (7)  | 0.0236 (8)  | 0.0206 (7)  | -0.0001 (6) | 0.0057 (6)  | 0.0004 (6)  |
| C16 | 0.0277 (9)  | 0.0297 (9)  | 0.0263 (8)  | -0.0070 (7) | 0.0070 (7)  | 0.0042 (7)  |
| C17 | 0.0345 (10) | 0.0516 (12) | 0.0187 (8)  | -0.0090 (8) | 0.0097 (7)  | -0.0082 (8) |
| C18 | 0.0289 (9)  | 0.0360 (11) | 0.0577 (13) | 0.0138 (8)  | 0.0180 (9)  | 0.0095 (9)  |

*Geometric parameters (Å, °)*

|            |              |              |             |
|------------|--------------|--------------|-------------|
| Sn—C11     | 2.4847 (4)   | C9—C10       | 1.384 (2)   |
| Sn—S1      | 2.4760 (4)   | C9—H9        | 0.9500      |
| Sn—S2      | 2.7409 (4)   | C10—H10      | 0.9500      |
| Sn—C11     | 2.1884 (14)  | C11—C12      | 1.522 (2)   |
| Sn—C15     | 2.1879 (15)  | C11—C14      | 1.523 (2)   |
| S1—C1      | 1.7470 (15)  | C11—C13      | 1.524 (2)   |
| S2—C1      | 1.7109 (15)  | C12—H12A     | 0.9800      |
| N1—C1      | 1.3240 (18)  | C12—H12B     | 0.9800      |
| N1—C4      | 1.4791 (18)  | C12—H12C     | 0.9800      |
| N1—C2      | 1.4839 (19)  | C13—H13A     | 0.9800      |
| C2—C3      | 1.523 (2)    | C13—H13B     | 0.9800      |
| C2—H2A     | 0.9900       | C13—H13C     | 0.9800      |
| C2—H2B     | 0.9900       | C14—H14A     | 0.9800      |
| C3—H3A     | 0.9800       | C14—H14B     | 0.9800      |
| C3—H3B     | 0.9800       | C14—H14C     | 0.9800      |
| C3—H3C     | 0.9800       | C15—C18      | 1.525 (2)   |
| C4—C5      | 1.509 (2)    | C15—C16      | 1.527 (2)   |
| C4—H4A     | 0.9900       | C15—C17      | 1.530 (2)   |
| C4—H4B     | 0.9900       | C16—H16A     | 0.9800      |
| C5—C10     | 1.390 (2)    | C16—H16B     | 0.9800      |
| C5—C6      | 1.390 (2)    | C16—H16C     | 0.9800      |
| C6—C7      | 1.391 (2)    | C17—H17A     | 0.9800      |
| C6—H6      | 0.9500       | C17—H17B     | 0.9800      |
| C7—C8      | 1.386 (2)    | C17—H17C     | 0.9800      |
| C7—H7      | 0.9500       | C18—H18A     | 0.9800      |
| C8—C9      | 1.386 (2)    | C18—H18B     | 0.9800      |
| C8—H8      | 0.9500       | C18—H18C     | 0.9800      |
| C15—Sn—C11 | 125.79 (6)   | C9—C10—C5    | 120.31 (14) |
| C15—Sn—S1  | 117.55 (4)   | C9—C10—H10   | 119.8       |
| C11—Sn—S1  | 115.59 (4)   | C5—C10—H10   | 119.8       |
| C15—Sn—C11 | 98.77 (4)    | C12—C11—C14  | 110.27 (15) |
| C11—Sn—C11 | 96.17 (4)    | C12—C11—C13  | 109.80 (14) |
| S1—Sn—C11  | 84.342 (12)  | C14—C11—C13  | 110.21 (14) |
| C15—Sn—S2  | 93.43 (4)    | C12—C11—Sn   | 108.21 (10) |
| C11—Sn—S2  | 96.04 (4)    | C14—C11—Sn   | 107.78 (10) |
| S1—Sn—S2   | 68.654 (12)  | C13—C11—Sn   | 110.52 (10) |
| C11—Sn—S2  | 152.989 (12) | C11—C12—H12A | 109.5       |

|              |             |                |             |
|--------------|-------------|----------------|-------------|
| C1—S1—Sn     | 91.00 (5)   | C11—C12—H12B   | 109.5       |
| C1—S2—Sn     | 83.22 (5)   | H12A—C12—H12B  | 109.5       |
| C1—N1—C4     | 122.17 (12) | C11—C12—H12C   | 109.5       |
| C1—N1—C2     | 121.73 (12) | H12A—C12—H12C  | 109.5       |
| C4—N1—C2     | 116.09 (11) | H12B—C12—H12C  | 109.5       |
| N1—C1—S2     | 123.80 (11) | C11—C13—H13A   | 109.5       |
| N1—C1—S1     | 119.10 (11) | C11—C13—H13B   | 109.5       |
| S2—C1—S1     | 117.10 (8)  | H13A—C13—H13B  | 109.5       |
| N1—C2—C3     | 113.75 (12) | C11—C13—H13C   | 109.5       |
| N1—C2—H2A    | 108.8       | H13A—C13—H13C  | 109.5       |
| C3—C2—H2A    | 108.8       | H13B—C13—H13C  | 109.5       |
| N1—C2—H2B    | 108.8       | C11—C14—H14A   | 109.5       |
| C3—C2—H2B    | 108.8       | C11—C14—H14B   | 109.5       |
| H2A—C2—H2B   | 107.7       | H14A—C14—H14B  | 109.5       |
| C2—C3—H3A    | 109.5       | C11—C14—H14C   | 109.5       |
| C2—C3—H3B    | 109.5       | H14A—C14—H14C  | 109.5       |
| H3A—C3—H3B   | 109.5       | H14B—C14—H14C  | 109.5       |
| C2—C3—H3C    | 109.5       | C18—C15—C16    | 110.55 (15) |
| H3A—C3—H3C   | 109.5       | C18—C15—C17    | 111.09 (15) |
| H3B—C3—H3C   | 109.5       | C16—C15—C17    | 109.57 (14) |
| N1—C4—C5     | 110.67 (12) | C18—C15—Sn     | 108.38 (11) |
| N1—C4—H4A    | 109.5       | C16—C15—Sn     | 108.51 (10) |
| C5—C4—H4A    | 109.5       | C17—C15—Sn     | 108.66 (10) |
| N1—C4—H4B    | 109.5       | C15—C16—H16A   | 109.5       |
| C5—C4—H4B    | 109.5       | C15—C16—H16B   | 109.5       |
| H4A—C4—H4B   | 108.1       | H16A—C16—H16B  | 109.5       |
| C10—C5—C6    | 119.24 (14) | C15—C16—H16C   | 109.5       |
| C10—C5—C4    | 119.60 (13) | H16A—C16—H16C  | 109.5       |
| C6—C5—C4     | 121.08 (14) | H16B—C16—H16C  | 109.5       |
| C5—C6—C7     | 120.61 (15) | C15—C17—H17A   | 109.5       |
| C5—C6—H6     | 119.7       | C15—C17—H17B   | 109.5       |
| C7—C6—H6     | 119.7       | H17A—C17—H17B  | 109.5       |
| C8—C7—C6     | 119.51 (15) | C15—C17—H17C   | 109.5       |
| C8—C7—H7     | 120.2       | H17A—C17—H17C  | 109.5       |
| C6—C7—H7     | 120.2       | H17B—C17—H17C  | 109.5       |
| C9—C8—C7     | 120.14 (15) | C15—C18—H18A   | 109.5       |
| C9—C8—H8     | 119.9       | C15—C18—H18B   | 109.5       |
| C7—C8—H8     | 119.9       | H18A—C18—H18B  | 109.5       |
| C10—C9—C8    | 120.15 (14) | C15—C18—H18C   | 109.5       |
| C10—C9—H9    | 119.9       | H18A—C18—H18C  | 109.5       |
| C8—C9—H9     | 119.9       | H18B—C18—H18C  | 109.5       |
|              |             |                |             |
| C15—Sn—S1—C1 | -83.40 (7)  | C8—C9—C10—C5   | 0.5 (2)     |
| C11—Sn—S1—C1 | 85.49 (6)   | C6—C5—C10—C9   | -2.0 (2)    |
| C11—Sn—S1—C1 | 179.64 (5)  | C4—C5—C10—C9   | 174.62 (14) |
| S2—Sn—S1—C1  | -0.96 (5)   | C15—Sn—C11—C12 | -55.53 (13) |
| C15—Sn—S2—C1 | 119.28 (6)  | S1—Sn—C11—C12  | 136.63 (11) |
| C11—Sn—S2—C1 | -114.17 (6) | C11—Sn—C11—C12 | 49.96 (11)  |

|              |              |                |              |
|--------------|--------------|----------------|--------------|
| S1—Sn—S2—C1  | 0.98 (5)     | S2—Sn—C11—C12  | -154.18 (11) |
| C11—Sn—S2—C1 | 2.29 (6)     | C15—Sn—C11—C14 | -174.77 (11) |
| C4—N1—C1—S2  | 0.84 (19)    | S1—Sn—C11—C14  | 17.39 (12)   |
| C2—N1—C1—S2  | 179.45 (10)  | C11—Sn—C11—C14 | -69.28 (11)  |
| C4—N1—C1—S1  | -179.25 (10) | S2—Sn—C11—C14  | 86.58 (11)   |
| C2—N1—C1—S1  | -0.64 (18)   | C15—Sn—C11—C13 | 64.74 (14)   |
| Sn—S2—C1—N1  | 178.46 (13)  | S1—Sn—C11—C13  | -103.11 (12) |
| Sn—S2—C1—S1  | -1.46 (7)    | C11—Sn—C11—C13 | 170.23 (12)  |
| Sn—S1—C1—N1  | -178.32 (11) | S2—Sn—C11—C13  | -33.91 (12)  |
| Sn—S1—C1—S2  | 1.60 (8)     | C11—Sn—C15—C18 | -171.31 (11) |
| C1—N1—C2—C3  | -82.33 (17)  | S1—Sn—C15—C18  | -3.68 (13)   |
| C4—N1—C2—C3  | 96.36 (15)   | C11—Sn—C15—C18 | 84.49 (12)   |
| C1—N1—C4—C5  | 117.52 (15)  | S2—Sn—C15—C18  | -71.34 (12)  |
| C2—N1—C4—C5  | -61.16 (16)  | C11—Sn—C15—C16 | -51.22 (13)  |
| N1—C4—C5—C10 | -67.27 (17)  | S1—Sn—C15—C16  | 116.41 (10)  |
| N1—C4—C5—C6  | 109.31 (16)  | C11—Sn—C15—C16 | -155.42 (10) |
| C10—C5—C6—C7 | 1.8 (2)      | S2—Sn—C15—C16  | 48.75 (11)   |
| C4—C5—C6—C7  | -174.75 (14) | C11—Sn—C15—C17 | 67.86 (14)   |
| C5—C6—C7—C8  | -0.2 (2)     | S1—Sn—C15—C17  | -124.51 (11) |
| C6—C7—C8—C9  | -1.4 (2)     | C11—Sn—C15—C17 | -36.34 (12)  |
| C7—C8—C9—C10 | 1.2 (2)      | S2—Sn—C15—C17  | 167.83 (12)  |

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C5–C10 ring.

| <i>D</i> —H $\cdots$ <i>A</i>      | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C3—H3a $\cdots$ Cg1                | 0.98        | 2.78                | 3.6491 (18)                | 149                           |
| C13—H13b $\cdots$ Cg1 <sup>i</sup> | 0.98        | 2.96                | 3.5401 (18)                | 119                           |

Symmetry code: (i)  $-x+1, -y, -z+1$ .