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## Structure Reports

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# $(\mu$ -Piperazine-1,4-dicarbodithioato- $\kappa^4 S, S', S'', S''')$ bis[triphenyltin(IV)] dichloromethane solvate

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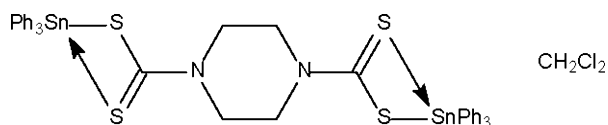
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 Key indicators: single-crystal X-ray study;  $T = 98$  K; mean  $\sigma(C-C) = 0.007$  Å; disorder in solvent or counterion;  $R$  factor = 0.049;  $wR$  factor = 0.113; data-to-parameter ratio = 18.0.

The dinuclear centrosymmetric title compound,  $[\text{Sn}_2(\text{C}_6\text{H}_5)_6(\text{C}_6\text{H}_8\text{N}_2\text{S}_4)] \cdot \text{CH}_2\text{Cl}_2$ , features a distorted *cis*-trigonal-bipyramidal coordination geometry for Sn based on a  $\text{C}_3\text{S}_2$  donor set. The dinuclear molecule lies across a centre of inversion. The solvent dichloromethane molecule is disordered about a centre of inversion.

## Related literature

For a review of tin dithiocarbamates, see: Tiekink (2008). For a related structure, see: Yin *et al.* (2002). For analysis of trigonal-bipyramidal geometries, see: Addison *et al.* (1984).



## Experimental

## Crystal data

 $[\text{Sn}_2(\text{C}_6\text{H}_5)_6(\text{C}_6\text{H}_8\text{N}_2\text{S}_4)] \cdot \text{CH}_2\text{Cl}_2$   
 $M_r = 1021.37$ 

 Monoclinic,  $P2_1/c$ 
 $a = 14.681$  (5) Å

 $b = 10.758$  (3) Å

 $c = 13.470$  (4) Å

 $\beta = 90.379$  (6)°

 $V = 2127.3$  (11) Å<sup>3</sup>
 $Z = 2$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.53$  mm<sup>-1</sup>
 $T = 98$  (2) K

 $0.35 \times 0.15 \times 0.01$  mm

## Data collection

 Rigaku AFC12 $\kappa$ /SATURN724 diffractometer

 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)

 $T_{\min} = 0.354$ ,  $T_{\max} = 1$ 

(expected range = 0.346–0.977)

14400 measured reflections

4389 independent reflections

 4021 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.048$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$ 
 $wR(F^2) = 0.113$ 
 $S = 1.10$ 

4389 reflections

244 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.77$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -1.12$  e Å<sup>-3</sup>

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2481).

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## supporting information

*Acta Cryst.* (2008). E64, m1177 [doi:10.1107/S1600536808025890]

**( $\mu$ -Piperazine-1,4-dicarbodithioato- $\kappa^4$ S,S':S'',S''')bis[triphenyltin(IV)] dichloromethane solvate**

**Pavel Poplaukhin and Edward R. T. Tiekink**

**S1. Comment**

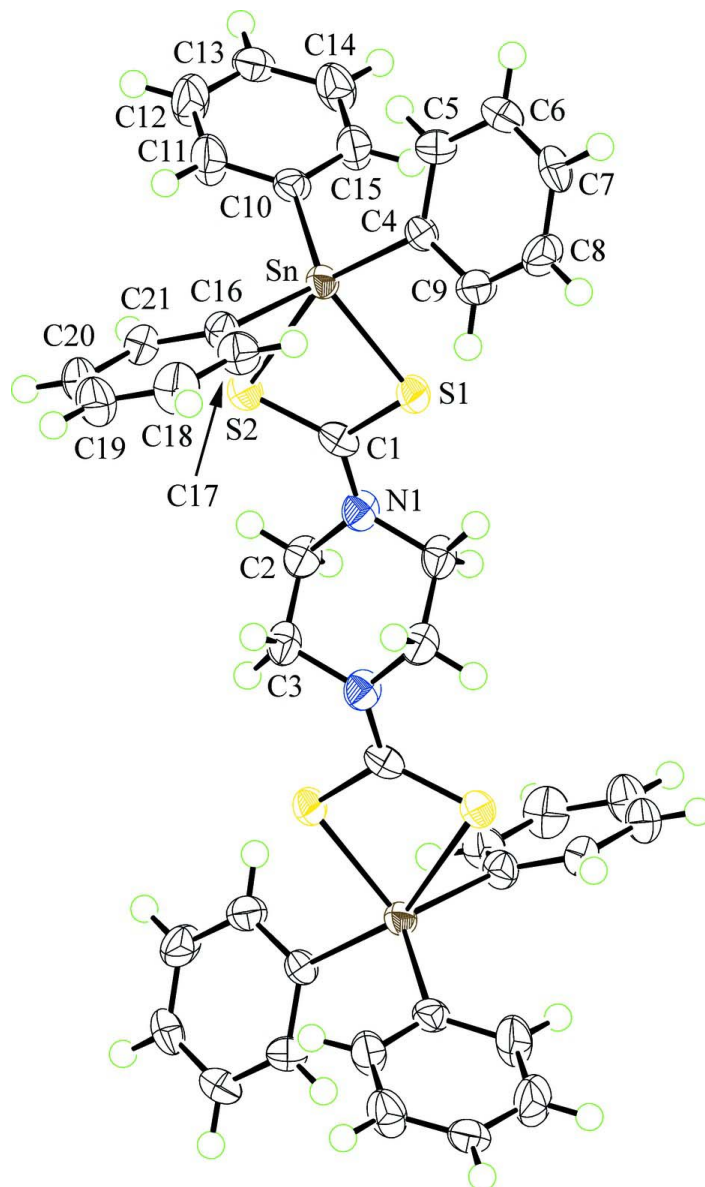
Tin dithiocarbamates continue to attract interest owing to their variety of applications (Tiekink, 2008). The title compound,  $\text{Ph}_3\text{SnS}_2\text{CN}(\text{CH}_2\text{CH}_2)_2\text{NCS}_2\text{SnPh}_3$ , has been reported previously as a methanol solvate (Yin *et al.*, 2002). The present structure (I) has been isolated as a dichloromethane solvate, Fig. 1. The molecule is centrosymmetric so that the  $\text{Ph}_3\text{Sn}$  entities lie to either side of the pyrrolidine ring which adopts a chair conformation. The dithiocarbamate ligand coordinates in an asymmetric mode, forming Sn—S1 and Sn—S2 distances of 2.4699 (13) and 3.0715 (13) Å, respectively. The coordination geometry is based on a distorted trigonal bipyramid as indicated by the value of  $\tau = 0.64$  (Addison *et al.*, 1984).

**S2. Experimental**

The title compound was prepared by following a literature procedure (Yin *et al.*, 2002). Colourless crystals were isolated by the slow evaporation of a dichloromethane solution of (I); m.p. 487–489 K (crystal turned opaque at 363–368 K). TGA: two steps, First mass loss 7.2% (onset 388.3 K, midpoint 392.6 K, endset 396.9 K) corresponds to loss  $\text{CH}_2\text{Cl}_2$  (8.2% theoretical). Second mass loss 69.3% (onset 558.5 K, midpoint 620 K, endset 680 K), corresponds to decomposition to SnS (total experimental mass loss 76.5% cf. theoretical value 70.5%). IR ( $\text{cm}^{-1}$ ): 1427, 1416 (strong, C=N), 1214 (strong, C—S).

**S3. Refinement**

The H atoms were geometrically placed (C—H = 0.95–0.99 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The solvent dichloromethane molecule was disordered about a centre of inversion and was modelled with anisotropic displacement parameters.

**Figure 1**

Molecular structure of (I) showing the crystallographic numbering scheme. Displacement ellipsoids are shown at the 70% probability level. Unlabelled atoms are related by the symmetry operation  $i: -x, 1-y, 1-z$ . The disordered dichloromethane molecule is omitted.

**( $\mu$ -Piperazine-1,4-dicarbodithio- $\kappa^4S,S':S'',S'''$ )bis[triphenyltin(IV)] dichloromethane solvate**

*Crystal data*

$[\text{Sn}_2(\text{C}_6\text{H}_5)_6(\text{C}_6\text{H}_8\text{N}_2\text{S}_4)] \cdot \text{CH}_2\text{Cl}_2$

$M_r = 1021.37$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 14.681(5)\ \text{\AA}$

$b = 10.758(3)\ \text{\AA}$

$c = 13.470(4)\ \text{\AA}$

$\beta = 90.379(6)^\circ$

$V = 2127.3(11)\ \text{\AA}^3$

$Z = 2$

$F(000) = 1020$

$D_x = 1.594\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71069\ \text{\AA}$

Cell parameters from 13756 reflections

$\theta = 2.4\text{--}40.7^\circ$   
 $\mu = 1.53\text{ mm}^{-1}$   
 $T = 98\text{ K}$

Plate, colourless  
 $0.35 \times 0.15 \times 0.02\text{ mm}$

*Data collection*

Rigaku AFC12 $\kappa$ /SATURN724  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.354$ ,  $T_{\max} = 1$

14400 measured reflections  
 4389 independent reflections  
 4021 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$   
 $\theta_{\max} = 26.5^\circ$ ,  $\theta_{\min} = 2.4^\circ$   
 $h = -17 \rightarrow 18$   
 $k = -13 \rightarrow 13$   
 $l = -16 \rightarrow 16$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.113$   
 $S = 1.10$   
 4389 reflections  
 244 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  
 $w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 8.4194P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.77\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.12\text{ e \AA}^{-3}$

*Special details*

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

**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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn	0.23132 (2)	0.37950 (3)	0.17164 (2)	0.02056 (11)	
S1	0.10733 (8)	0.32408 (10)	0.28651 (9)	0.0237 (3)	
S2	0.12861 (8)	0.59723 (11)	0.26696 (9)	0.0244 (3)	
N1	0.0190 (3)	0.4872 (4)	0.3970 (3)	0.0250 (9)	
C1	0.0795 (3)	0.4757 (4)	0.3239 (3)	0.0228 (9)	
C2	-0.0077 (3)	0.6087 (4)	0.4381 (4)	0.0264 (11)	
H2A	-0.0745	0.6193	0.4320	0.032*	
H2B	0.0220	0.6761	0.4002	0.032*	
C3	0.0208 (3)	0.6161 (4)	0.5471 (4)	0.0260 (10)	
H3A	0.0880	0.6128	0.5525	0.031*	
H3B	0.0001	0.6961	0.5756	0.031*	
C4	0.2559 (3)	0.1881 (4)	0.1326 (3)	0.0212 (9)	
C5	0.2678 (3)	0.1546 (5)	0.0335 (4)	0.0238 (10)	

H5	0.2690	0.2174	-0.0160	0.029*	
C6	0.2780 (3)	0.0316 (5)	0.0060 (4)	0.0284 (11)	
H6	0.2846	0.0103	-0.0620	0.034*	
C7	0.2785 (3)	-0.0610 (4)	0.0782 (4)	0.0284 (11)	
H7	0.2869	-0.1453	0.0596	0.034*	
C8	0.2666 (4)	-0.0303 (5)	0.1768 (4)	0.0320 (12)	
H8	0.2664	-0.0936	0.2259	0.038*	
C9	0.2549 (3)	0.0934 (4)	0.2042 (4)	0.0270 (10)	
H9	0.2462	0.1139	0.2721	0.032*	
C10	0.1869 (3)	0.4710 (4)	0.0402 (3)	0.0231 (10)	
C11	0.2262 (4)	0.5821 (5)	0.0088 (4)	0.0413 (14)	
H11	0.2767	0.6157	0.0442	0.050*	
C12	0.1920 (4)	0.6440 (5)	-0.0742 (5)	0.0424 (15)	
H12	0.2184	0.7205	-0.0944	0.051*	
C13	0.1199 (4)	0.5948 (4)	-0.1273 (4)	0.0272 (10)	
H13	0.0966	0.6377	-0.1836	0.033*	
C14	0.0818 (4)	0.4841 (5)	-0.0989 (4)	0.0344 (12)	
H14	0.0324	0.4497	-0.1356	0.041*	
C15	0.1166 (4)	0.4223 (5)	-0.0151 (4)	0.0307 (11)	
H15	0.0908	0.3449	0.0038	0.037*	
C16	0.3474 (3)	0.4550 (4)	0.2475 (4)	0.0238 (10)	
C17	0.4094 (3)	0.3737 (5)	0.2921 (4)	0.0297 (11)	
H17	0.4011	0.2865	0.2860	0.036*	
C18	0.4830 (4)	0.4199 (5)	0.3453 (4)	0.0369 (12)	
H18	0.5247	0.3640	0.3759	0.044*	
C19	0.4966 (4)	0.5477 (5)	0.3543 (4)	0.0378 (13)	
H19	0.5475	0.5791	0.3904	0.045*	
C20	0.4352 (3)	0.6280 (5)	0.3103 (4)	0.0308 (11)	
H20	0.4439	0.7151	0.3165	0.037*	
C21	0.3608 (3)	0.5833 (4)	0.2570 (4)	0.0247 (10)	
H21	0.3191	0.6397	0.2270	0.030*	
C22	0.5409 (12)	0.0134 (14)	0.5721 (11)	0.066 (4)	0.50
H22A	0.6046	0.0434	0.5764	0.080*	0.50
H22B	0.5172	0.0006	0.6400	0.080*	0.50
Cl1	0.4667 (2)	0.1259 (2)	0.4994 (2)	0.0958 (9)	

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn	0.02652 (19)	0.01628 (17)	0.01887 (18)	-0.00089 (12)	-0.00114 (13)	0.00000 (11)
S1	0.0281 (6)	0.0167 (5)	0.0263 (6)	-0.0002 (4)	0.0029 (5)	-0.0026 (4)
S2	0.0294 (6)	0.0191 (5)	0.0247 (6)	0.0000 (5)	0.0020 (5)	-0.0025 (4)
N1	0.027 (2)	0.0180 (19)	0.030 (2)	0.0038 (16)	0.0035 (17)	0.0006 (16)
C1	0.024 (2)	0.023 (2)	0.021 (2)	0.0046 (18)	-0.0024 (18)	-0.0055 (18)
C2	0.025 (2)	0.019 (2)	0.035 (3)	0.0045 (18)	0.010 (2)	-0.0009 (19)
C3	0.024 (2)	0.018 (2)	0.036 (3)	0.0017 (18)	0.007 (2)	-0.001 (2)
C4	0.026 (2)	0.015 (2)	0.023 (2)	0.0014 (17)	0.0030 (18)	-0.0032 (17)
C5	0.024 (2)	0.027 (2)	0.021 (2)	0.0037 (19)	0.0010 (18)	-0.0005 (19)

C6	0.032 (3)	0.030 (3)	0.023 (3)	0.001 (2)	-0.001 (2)	-0.008 (2)
C7	0.029 (3)	0.018 (2)	0.038 (3)	-0.0012 (19)	-0.002 (2)	-0.007 (2)
C8	0.043 (3)	0.021 (2)	0.032 (3)	0.001 (2)	0.007 (2)	0.006 (2)
C9	0.035 (3)	0.024 (2)	0.022 (2)	0.001 (2)	0.003 (2)	0.0007 (19)
C10	0.032 (2)	0.018 (2)	0.019 (2)	0.0025 (18)	0.0003 (19)	-0.0009 (17)
C11	0.057 (4)	0.033 (3)	0.034 (3)	-0.019 (3)	-0.024 (3)	0.012 (2)
C12	0.060 (4)	0.029 (3)	0.039 (3)	-0.014 (3)	-0.013 (3)	0.013 (2)
C13	0.041 (3)	0.022 (2)	0.019 (2)	0.006 (2)	-0.001 (2)	-0.0006 (19)
C14	0.039 (3)	0.029 (3)	0.035 (3)	-0.004 (2)	-0.016 (2)	0.002 (2)
C15	0.038 (3)	0.024 (2)	0.030 (3)	-0.007 (2)	-0.009 (2)	0.003 (2)
C16	0.018 (2)	0.027 (2)	0.026 (3)	-0.0031 (18)	-0.0007 (18)	-0.0023 (19)
C17	0.028 (3)	0.031 (3)	0.030 (3)	0.001 (2)	-0.004 (2)	0.001 (2)
C18	0.029 (3)	0.036 (3)	0.045 (3)	0.002 (2)	-0.006 (2)	0.004 (3)
C19	0.032 (3)	0.040 (3)	0.041 (3)	-0.011 (2)	-0.005 (2)	-0.005 (3)
C20	0.026 (3)	0.032 (3)	0.034 (3)	-0.009 (2)	-0.002 (2)	-0.003 (2)
C21	0.023 (2)	0.023 (2)	0.027 (3)	-0.0027 (19)	0.0017 (19)	0.0021 (19)
C22	0.102 (12)	0.050 (8)	0.048 (9)	0.001 (8)	0.023 (8)	0.001 (7)
C11	0.155 (3)	0.0477 (11)	0.0854 (17)	0.0173 (13)	0.0274 (17)	0.0024 (11)

*Geometric parameters (Å, °)*

Sn—C10	2.125 (5)	C10—C15	1.373 (7)
Sn—C16	2.141 (5)	C10—C11	1.394 (7)
Sn—C4	2.157 (4)	C11—C12	1.392 (8)
Sn—S1	2.4699 (13)	C11—H11	0.9500
Sn—S2	3.0715 (13)	C12—C13	1.378 (8)
S1—C1	1.756 (5)	C12—H12	0.9500
S2—C1	1.680 (5)	C13—C14	1.370 (7)
N1—C1	1.337 (6)	C13—H13	0.9500
N1—C3 <sup>i</sup>	1.466 (6)	C14—C15	1.403 (7)
N1—C2	1.473 (6)	C14—H14	0.9500
C2—C3	1.527 (7)	C15—H15	0.9500
C2—H2A	0.9900	C16—C17	1.396 (7)
C2—H2B	0.9900	C16—C21	1.400 (7)
C3—N1 <sup>i</sup>	1.466 (6)	C17—C18	1.385 (7)
C3—H3A	0.9900	C17—H17	0.9500
C3—H3B	0.9900	C18—C19	1.395 (8)
C4—C5	1.394 (6)	C18—H18	0.9500
C4—C9	1.403 (7)	C19—C20	1.380 (8)
C5—C6	1.382 (7)	C19—H19	0.9500
C5—H5	0.9500	C20—C21	1.389 (7)
C6—C7	1.392 (7)	C20—H20	0.9500
C6—H6	0.9500	C21—H21	0.9500
C7—C8	1.380 (7)	C22—C11 <sup>ii</sup>	1.784 (15)
C7—H7	0.9500	C22—C11	1.896 (16)
C8—C9	1.392 (7)	C22—H22A	0.9900
C8—H8	0.9500	C22—H22B	0.9900
C9—H9	0.9500	C11—C22 <sup>ii</sup>	1.784 (15)

C10—Sn—C16	117.43 (18)	C8—C9—H9	119.7
C10—Sn—C4	106.86 (18)	C4—C9—H9	119.7
C16—Sn—C4	110.16 (18)	C15—C10—C11	118.3 (5)
C10—Sn—S1	114.23 (13)	C15—C10—Sn	120.1 (4)
C16—Sn—S1	112.36 (13)	C11—C10—Sn	121.7 (4)
C4—Sn—S1	92.74 (12)	C12—C11—C10	120.4 (5)
C10—Sn—S2	81.15 (12)	C12—C11—H11	119.8
C16—Sn—S2	84.41 (13)	C10—C11—H11	119.8
C4—Sn—S2	156.03 (12)	C13—C12—C11	120.3 (5)
S1—Sn—S2	63.66 (4)	C13—C12—H12	119.9
C1—S1—Sn	97.41 (16)	C11—C12—H12	119.9
C1—S2—Sn	79.09 (16)	C14—C13—C12	120.2 (5)
C1—N1—C3 <sup>i</sup>	125.3 (4)	C14—C13—H13	119.9
C1—N1—C2	122.6 (4)	C12—C13—H13	119.9
C3 <sup>i</sup> —N1—C2	111.8 (4)	C13—C14—C15	119.3 (5)
N1—C1—S2	123.6 (4)	C13—C14—H14	120.4
N1—C1—S1	117.0 (4)	C15—C14—H14	120.4
S2—C1—S1	119.4 (3)	C10—C15—C14	121.6 (5)
N1—C2—C3	109.6 (4)	C10—C15—H15	119.2
N1—C2—H2A	109.7	C14—C15—H15	119.2
C3—C2—H2A	109.7	C17—C16—C21	119.2 (5)
N1—C2—H2B	109.7	C17—C16—Sn	118.9 (4)
C3—C2—H2B	109.7	C21—C16—Sn	121.9 (4)
H2A—C2—H2B	108.2	C18—C17—C16	120.2 (5)
N1 <sup>i</sup> —C3—C2	110.3 (4)	C18—C17—H17	119.9
N1 <sup>i</sup> —C3—H3A	109.6	C16—C17—H17	119.9
C2—C3—H3A	109.6	C17—C18—C19	120.6 (5)
N1 <sup>i</sup> —C3—H3B	109.6	C17—C18—H18	119.7
C2—C3—H3B	109.6	C19—C18—H18	119.7
H3A—C3—H3B	108.1	C20—C19—C18	119.1 (5)
C5—C4—C9	118.2 (4)	C20—C19—H19	120.4
C5—C4—Sn	120.2 (3)	C18—C19—H19	120.4
C9—C4—Sn	121.5 (3)	C19—C20—C21	121.0 (5)
C6—C5—C4	121.2 (5)	C19—C20—H20	119.5
C6—C5—H5	119.4	C21—C20—H20	119.5
C4—C5—H5	119.4	C20—C21—C16	119.8 (5)
C5—C6—C7	119.8 (5)	C20—C21—H21	120.1
C5—C6—H6	120.1	C16—C21—H21	120.1
C7—C6—H6	120.1	C11 <sup>ii</sup> —C22—C11	102.9 (8)
C8—C7—C6	120.1 (5)	C11 <sup>ii</sup> —C22—H22A	111.2
C8—C7—H7	120.0	C11—C22—H22A	111.2
C6—C7—H7	120.0	C11 <sup>ii</sup> —C22—H22B	111.2
C7—C8—C9	120.0 (5)	C11—C22—H22B	111.2
C7—C8—H8	120.0	H22A—C22—H22B	109.1
C9—C8—H8	120.0	C22 <sup>ii</sup> —C11—C22	77.1 (8)
C8—C9—C4	120.6 (5)		

C10—Sn—S1—C1	-69.6 (2)	Sn—C4—C9—C8	176.9 (4)
C16—Sn—S1—C1	67.4 (2)	C16—Sn—C10—C15	175.8 (4)
C4—Sn—S1—C1	-179.5 (2)	C4—Sn—C10—C15	51.5 (4)
S2—Sn—S1—C1	-3.88 (16)	S1—Sn—C10—C15	-49.5 (4)
C10—Sn—S2—C1	126.8 (2)	S2—Sn—C10—C15	-105.3 (4)
C16—Sn—S2—C1	-114.3 (2)	C16—Sn—C10—C11	-5.6 (5)
C4—Sn—S2—C1	15.0 (4)	C4—Sn—C10—C11	-129.8 (5)
S1—Sn—S2—C1	4.10 (17)	S1—Sn—C10—C11	129.2 (4)
C3 <sup>i</sup> —N1—C1—S2	-175.8 (4)	S2—Sn—C10—C11	73.4 (4)
C2—N1—C1—S2	-2.8 (7)	C15—C10—C11—C12	2.7 (9)
C3 <sup>i</sup> —N1—C1—S1	4.6 (7)	Sn—C10—C11—C12	-176.0 (5)
C2—N1—C1—S1	177.6 (4)	C10—C11—C12—C13	-1.2 (10)
Sn—S2—C1—N1	174.5 (4)	C11—C12—C13—C14	-0.4 (9)
Sn—S2—C1—S1	-5.9 (2)	C12—C13—C14—C15	0.5 (8)
Sn—S1—C1—N1	-173.0 (3)	C11—C10—C15—C14	-2.6 (8)
Sn—S1—C1—S2	7.3 (3)	Sn—C10—C15—C14	176.1 (4)
C1—N1—C2—C3	-116.5 (5)	C13—C14—C15—C10	1.1 (8)
C3 <sup>i</sup> —N1—C2—C3	57.4 (5)	C10—Sn—C16—C17	-143.2 (4)
N1—C2—C3—N1 <sup>i</sup>	-56.4 (5)	C4—Sn—C16—C17	-20.6 (4)
C10—Sn—C4—C5	18.7 (4)	S1—Sn—C16—C17	81.2 (4)
C16—Sn—C4—C5	-110.0 (4)	S2—Sn—C16—C17	139.8 (4)
S1—Sn—C4—C5	135.0 (4)	C10—Sn—C16—C21	39.4 (5)
S2—Sn—C4—C5	125.3 (3)	C4—Sn—C16—C21	162.0 (4)
C10—Sn—C4—C9	-157.4 (4)	S1—Sn—C16—C21	-96.1 (4)
C16—Sn—C4—C9	74.0 (4)	S2—Sn—C16—C21	-37.6 (4)
S1—Sn—C4—C9	-41.1 (4)	C21—C16—C17—C18	0.2 (8)
S2—Sn—C4—C9	-50.8 (6)	Sn—C16—C17—C18	-177.2 (4)
C9—C4—C5—C6	0.3 (7)	C16—C17—C18—C19	-0.5 (9)
Sn—C4—C5—C6	-175.9 (4)	C17—C18—C19—C20	0.6 (9)
C4—C5—C6—C7	-1.4 (7)	C18—C19—C20—C21	-0.4 (9)
C5—C6—C7—C8	1.6 (8)	C19—C20—C21—C16	0.0 (8)
C6—C7—C8—C9	-0.5 (8)	C17—C16—C21—C20	0.0 (7)
C7—C8—C9—C4	-0.6 (8)	Sn—C16—C21—C20	177.4 (4)
C5—C4—C9—C8	0.7 (7)	C11 <sup>ii</sup> —C22—C11—C22 <sup>ii</sup>	0.000 (2)

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