

## A diorganotin(IV) complex with pyrazine-2-carbaldehyde 4-ethylthiosemicarbazone

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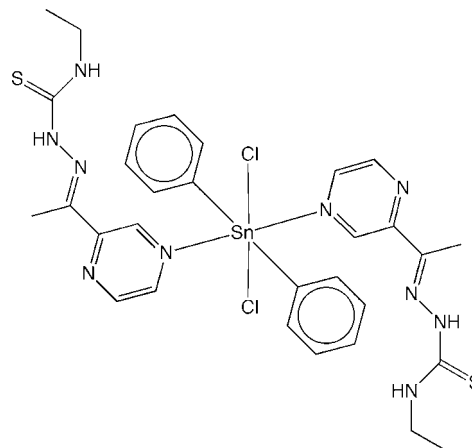
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Key indicators: single-crystal X-ray study;  $T = 90$  K; mean  $\sigma(C-C) = 0.002$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.071; data-to-parameter ratio = 34.9.

The reaction of pyrazine-2-carbaldehyde 4-ethylthiosemicarbazone (Hapetsc) with diphenyltin(IV) dichloride in ethanol resulted in the formation of the title compound, dichloridodiphenylbis(pyrazine-2-carbaldehyde 4-ethylthiosemicarbazone)tin(IV),  $[\text{Sn}(\text{C}_6\text{H}_5)_2\text{Cl}_2(\text{C}_9\text{H}_{13}\text{N}_5\text{S})_2]$ . The complex exhibits a distorted octahedron about the Sn atom, which lies on an inversion center and is coordinated by two Cl atoms, two phenyl ligands and two Hapetsc units. The pyrazine ligands are in a *trans* configuration and behave as monodentate donors through their ring N atoms. The Sn–Cl distances are 2.5484 (4) Å, the Sn–C distances are 2.1378 (12) Å and the Sn–N distances are 2.4032 (11) Å. One NH group of the thiosemicarbazone ligand forms an intramolecular S(5) hydrogen bond with an adjacent N atom on the same ligand. The other N–H group is not involved in hydrogen bonding.

### Related literature

For related literature, see: Ali & Livingstone (1974); Allen *et al.* (1979); Bamgboye & Bamgboye (1988); Barbieri *et al.* (1993); Campbell (1975); Casas *et al.* (1994, 1996, 1997); Davies (1998); De Sousa *et al.* (2001); Dey *et al.* (2003); Etter (1990); Padhye & Kauffman (1985); Venkatraman *et al.* (2004).



### Experimental

#### Crystal data

$[\text{Sn}(\text{C}_6\text{H}_5)_2\text{Cl}_2(\text{C}_9\text{H}_{13}\text{N}_5\text{S})_2]$   
 $M_r = 790.40$   
 Monoclinic,  $P2_1/c$   
 $a = 10.7262$  (15) Å  
 $b = 17.971$  (3) Å  
 $c = 9.0868$  (13) Å  
 $\beta = 109.641$  (6)°

$V = 1649.7$  (4) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.10$  mm<sup>-1</sup>  
 $T = 90$  K  
 0.27 × 0.22 × 0.20 mm

#### Data collection

Nonius KappaCCD diffractometer  
 (with Oxford Cryosystems  
 Cryostream cooler)  
 Absorption correction: multi-scan  
 (SCALEPACK; Otwinowski &

Minor, 1997)  
 $T_{\min} = 0.755$ ,  $T_{\max} = 0.810$   
 24456 measured reflections  
 7475 independent reflections  
 6422 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.071$   
 $S = 1.02$   
 7475 reflections  
 214 parameters

H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $\Delta\rho_{\max} = 0.85$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.29$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N5}-\text{H5N}\cdots\text{N3}$	0.91 (2)	2.16 (2)	2.6093 (17)	109.8 (16)

Data collection: COLLECT (Nonius, 2000); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2159).

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**supplementary materials**

*Acta Cryst.* (2007). E63, m2212-m2213 [ doi:10.1107/S1600536807035052 ]

## A diorganotin(IV) complex with pyrazine-2-carbaldehyde 4-ethylthiosemicarbazone

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### Comment

There has been a steady growth of interest in the synthesis, structure and reactivity studies of metal complexes of heterocyclic thiosemicarbazones due to their biological and pharmacological properties (Ali & Livingstone, 1974; Campbell, 1975; Padhye & Kauffman, 1985). The unique feature is attributed to the tautomeric equilibrium present in the thiosemicarbazone moiety and thereby the coordinating ability with many metal ions. Among the non-transition metals, organotin(IV) derivatives are of special interest due to environmental, and medical issues (Barbieri *et al.*, 1993; Bamgboye & Bamgboye, 1988; Casas *et al.*, 1994, Casas *et al.*, 1996, De Sousa *et al.*, 2001). Continuing with this type of studies, we describe here the structure of a diphenyltin dichloride derivative of pyrazine-2-carbaldehyde *N*(4)-ethyl-3-thiosemicarbazone (I).

The tin atom of the diphenyl dichloride unit lies on an inversion center, and is coordinated in monodentate fashion by the pyrazine nitrogen atoms of two thiosemicarbazone ligands, unlike the normal bidentate/tridentate modes of coordination. The yellow-colored complex is built up of discrete molecules of acetylpyrazine thiosemicarbazone ligand with diphenyl tin dichloride with the two chlorine atoms and two phenyl groups occupying the four equatorial positions (*trans* to each other) of a distorted octahedron around the tin atom. The pyrazine groups are in the inverse position and *trans* to one another. The angles subtended by the adjacent atoms to tin are 89.75 (4)°, [C10—Sn—Cl1], 88.99 (4)° [N1—Sn1—C10] and 91.79 (3)° (N1—Sn1—Cl1) and the corresponding bond distances are Sn—C [2.1378 (12)], Sn—Cl [2.5483 (4)] and Sn—N [2.4033 (11) Å]. The Sn—N bond length value is in the range of 2.27 to 2.58, and is less than the van der Waals radii of the two atoms, 3.74 Å (Allen *et al.*, 1979). The Sn—Cl bond is in the range of normal covalent radii (2.37–2.60 Å) (Casas *et al.*, 1997, Davies, 1998). The bond length Sn—C (phenyl) is slightly shorter compared to the tin adduct reported 2.1424 (14) Å by us earlier (Venkatraman *et al.*, 2004). The bond length Sn—C increases with an increase in coordination number from four [2.122 (11) Å] (in Ph<sub>2</sub>SnCl<sub>2</sub>) and higher as expected (Dey *et al.*, 2003).

N—H groups usually serve as hydrogen-bond donors, however, no intermolecular hydrogen bonding is present in this structure. N—H group N5 forms an intramolecular hydrogen bond of graph set designation S(5) (Etter, 1990), with N3 as acceptor, N3···N5 2.609 (2) Å. In five-membered rings, the hydrogen-bonding geometry necessarily distorts greatly from linearity. The H···N3 distance is 2.15 (2) Å, and the angle about H is 109.9 (19)°. The other N—H group N4 is not involved in hydrogen bonding.

### Experimental

The tin complex of acetylpyrazine *N*(4)-ethylthiosemicarbazone was prepared by the following procedure: a solution of diphenyltin dichloride (0.69 g, 2 mmol) in 20 ml of dry methanol was added to a refluxing methanol solution (20 ml) of the ligand. The resulting mixture was refluxed for 1 h. Cooling followed by slow evaporation at room temperature produced yellow crystals (*ca* 75% yield), with a melting point 459–461 K. IR spectra were obtained in the 4000–400 cm<sup>-1</sup> range in KBr pellets on a Nicolet 670 FT—IR spectrophotometer  $\nu_{\text{N—H}}$  3350,  $\nu_{\text{C—N}}$  1590, 1530(*s*),  $\nu_{\text{C—S}}$  850(*s*) cm<sup>-1</sup>.

## Refinement

H atoms on C were placed in idealized positions with C—H distances 0.95–0.99 Å and thereafter treated as riding.  $U_{\text{iso}}$  for H was assigned as 1.2 times  $U_{\text{eq}}$  of the attached C or N atoms (1.5 for methyl). A torsional parameter was refined for each methyl group. N—H hydrogen atom positions were refined.

## Figures

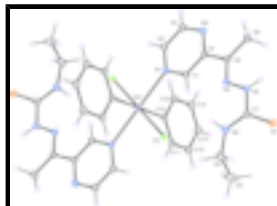


Fig. 1. Numbering scheme and displacement ellipsoids at the 50% level. H atoms are represented with arbitrary radius. Unlabelled atoms are related by the symmetry operation  $(1 - x, 1 - y, 1 - z)$ .

## dichloridodiphenylbis(pyrazine-2-carbaldehyde 4-ethylthiosemicarbazone)tin(IV)

### Crystal data

$[\text{Sn}(\text{C}_6\text{H}_5)_2\text{Cl}_2(\text{C}_9\text{H}_{13}\text{N}_5\text{S})_2]$

$M_r = 790.40$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 10.7262\ (15)\ \text{\AA}$

$b = 17.971\ (3)\ \text{\AA}$

$c = 9.0868\ (13)\ \text{\AA}$

$\beta = 109.641\ (6)^\circ$

$V = 1649.7\ (4)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 804$

$D_x = 1.591\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6430 reflections

$\theta = 2.5\text{--}35.6^\circ$

$\mu = 1.10\ \text{mm}^{-1}$

$T = 90\ \text{K}$

Needle fragment, yellow

$0.27 \times 0.22 \times 0.20\ \text{mm}$

### Data collection

Nonius KappaCCD (with Oxford Cryosystems Cryo-stream cooler) diffractometer

7475 independent reflections

Radiation source: fine-focus sealed tube

6422 reflections with  $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.026$

$T = 90\ \text{K}$

$\theta_{\text{max}} = 35.6^\circ$

$\omega$  scans with  $\kappa$  offsets

$\theta_{\text{min}} = 2.7^\circ$

Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)

$h = -17 \rightarrow 17$

$T_{\text{min}} = 0.755$ ,  $T_{\text{max}} = 0.810$

$k = -25 \rightarrow 29$

24456 measured reflections

$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2 + 1.1288P]$
$wR(F^2) = 0.071$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\max} = 0.001$
7475 reflections	$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$
214 parameters	$\Delta\rho_{\min} = -1.29 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0022 (4)

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	0.5000	0.5000	0.00677 (3)
Cl1	0.42470 (3)	0.606662 (17)	0.63487 (3)	0.01054 (6)
S1	-0.15561 (4)	0.75620 (2)	0.60254 (4)	0.01438 (7)
N1	0.27549 (11)	0.46903 (6)	0.34850 (13)	0.00969 (18)
N2	0.00894 (12)	0.45016 (7)	0.16677 (14)	0.0129 (2)
N3	-0.01068 (11)	0.59622 (6)	0.42005 (13)	0.01122 (19)
N4	-0.09760 (11)	0.64282 (7)	0.45362 (14)	0.01177 (19)
H4N	-0.176 (2)	0.6485 (12)	0.391 (2)	0.014*
N5	0.07887 (12)	0.68918 (7)	0.65242 (15)	0.0152 (2)
H5N	0.123 (2)	0.6529 (13)	0.620 (3)	0.018*
C1	0.18071 (13)	0.51177 (7)	0.36914 (16)	0.0111 (2)
H1	0.2044	0.5495	0.4468	0.013*
C2	0.23751 (13)	0.41575 (8)	0.23804 (16)	0.0121 (2)
H2	0.3020	0.3837	0.2214	0.015*
C3	0.10492 (14)	0.40721 (8)	0.14829 (16)	0.0137 (2)

## supplementary materials

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H3	0.0813	0.3694	0.0707	0.016*
C4	0.04715 (13)	0.50219 (7)	0.27881 (15)	0.00994 (19)
C5	-0.05560 (13)	0.55018 (7)	0.30524 (15)	0.0105 (2)
C6	-0.19717 (13)	0.54186 (8)	0.20520 (17)	0.0146 (2)
H6A	-0.2495	0.5267	0.2701	0.022*
H6B	-0.2045	0.5040	0.1251	0.022*
H6C	-0.2304	0.5895	0.1547	0.022*
C7	-0.04970 (13)	0.69445 (7)	0.57094 (15)	0.0115 (2)
C8	0.14983 (16)	0.73660 (10)	0.78438 (18)	0.0208 (3)
H8A	0.2195	0.7070	0.8615	0.025*
H8B	0.0875	0.7544	0.8360	0.025*
C9	0.21281 (19)	0.80299 (11)	0.7342 (2)	0.0301 (4)
H9A	0.2716	0.7857	0.6788	0.045*
H9B	0.2641	0.8316	0.8266	0.045*
H9C	0.1435	0.8347	0.6647	0.045*
C10	0.50493 (12)	0.57431 (7)	0.31832 (14)	0.00910 (19)
C11	0.56171 (13)	0.64482 (7)	0.35463 (15)	0.0107 (2)
H11	0.5983	0.6599	0.4607	0.013*
C12	0.56497 (14)	0.69314 (8)	0.23604 (16)	0.0137 (2)
H12	0.6054	0.7406	0.2616	0.016*
C13	0.50916 (14)	0.67200 (8)	0.08006 (16)	0.0140 (2)
H13	0.5104	0.7052	-0.0007	0.017*
C14	0.45164 (14)	0.60209 (8)	0.04319 (15)	0.0130 (2)
H14	0.4130	0.5877	-0.0631	0.016*
C15	0.45039 (13)	0.55302 (7)	0.16182 (15)	0.0109 (2)
H15	0.4123	0.5050	0.1360	0.013*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.00730 (5)	0.00772 (5)	0.00631 (5)	0.00094 (4)	0.00365 (3)	0.00064 (4)
Cl1	0.01262 (12)	0.01062 (12)	0.00942 (11)	0.00198 (10)	0.00508 (9)	-0.00091 (9)
S1	0.01682 (15)	0.01227 (14)	0.01643 (14)	0.00014 (11)	0.00872 (12)	-0.00298 (11)
N1	0.0089 (4)	0.0106 (4)	0.0103 (4)	0.0001 (3)	0.0041 (3)	0.0003 (3)
N2	0.0121 (5)	0.0136 (5)	0.0128 (5)	-0.0004 (4)	0.0039 (4)	-0.0032 (4)
N3	0.0109 (4)	0.0112 (4)	0.0123 (4)	0.0007 (4)	0.0049 (4)	-0.0014 (4)
N4	0.0098 (4)	0.0125 (5)	0.0130 (5)	0.0012 (4)	0.0038 (4)	-0.0025 (4)
N5	0.0126 (5)	0.0169 (5)	0.0145 (5)	-0.0002 (4)	0.0025 (4)	-0.0044 (4)
C1	0.0097 (5)	0.0118 (5)	0.0122 (5)	-0.0002 (4)	0.0042 (4)	-0.0017 (4)
C2	0.0110 (5)	0.0130 (5)	0.0131 (5)	0.0006 (4)	0.0049 (4)	-0.0017 (4)
C3	0.0134 (5)	0.0137 (5)	0.0140 (5)	-0.0002 (4)	0.0046 (4)	-0.0040 (4)
C4	0.0085 (5)	0.0112 (5)	0.0107 (5)	-0.0003 (4)	0.0041 (4)	-0.0006 (4)
C5	0.0088 (5)	0.0113 (5)	0.0118 (5)	-0.0003 (4)	0.0038 (4)	-0.0006 (4)
C6	0.0085 (5)	0.0168 (6)	0.0174 (6)	-0.0003 (4)	0.0028 (4)	-0.0041 (5)
C7	0.0136 (5)	0.0115 (5)	0.0108 (5)	-0.0015 (4)	0.0059 (4)	-0.0004 (4)
C8	0.0179 (6)	0.0256 (7)	0.0158 (6)	-0.0010 (6)	0.0014 (5)	-0.0078 (5)
C9	0.0241 (8)	0.0331 (9)	0.0333 (9)	-0.0137 (7)	0.0102 (7)	-0.0156 (8)
C10	0.0095 (5)	0.0102 (5)	0.0087 (5)	0.0006 (4)	0.0045 (4)	0.0014 (4)

C11	0.0112 (5)	0.0103 (5)	0.0119 (5)	0.0003 (4)	0.0053 (4)	0.0007 (4)
C12	0.0156 (6)	0.0120 (5)	0.0154 (6)	-0.0008 (4)	0.0076 (5)	0.0022 (4)
C13	0.0155 (6)	0.0154 (6)	0.0130 (5)	0.0010 (5)	0.0072 (4)	0.0049 (4)
C14	0.0147 (5)	0.0163 (6)	0.0089 (5)	0.0000 (5)	0.0051 (4)	0.0018 (4)
C15	0.0117 (5)	0.0127 (5)	0.0088 (5)	-0.0007 (4)	0.0043 (4)	0.0006 (4)

*Geometric parameters (Å, °)*

Sn1—C10 <sup>i</sup>	2.1378 (12)	C4—C5	1.4813 (18)
Sn1—C10	2.1378 (12)	C5—C6	1.4921 (19)
Sn1—N1 <sup>i</sup>	2.4032 (11)	C6—H6A	0.9800
Sn1—N1	2.4033 (11)	C6—H6B	0.9800
Sn1—Cl1 <sup>i</sup>	2.5483 (4)	C6—H6C	0.9800
Sn1—Cl1	2.5483 (4)	C8—C9	1.515 (3)
S1—C7	1.6804 (14)	C8—H8A	0.9900
N1—C1	1.3367 (17)	C8—H8B	0.9900
N1—C2	1.3473 (17)	C9—H9A	0.9800
N2—C4	1.3411 (17)	C9—H9B	0.9800
N2—C3	1.3416 (18)	C9—H9C	0.9800
N3—C5	1.2912 (17)	C10—C11	1.3966 (18)
N3—N4	1.3619 (16)	C10—C15	1.3971 (18)
N4—C7	1.3759 (17)	C11—C12	1.3934 (18)
N4—H4N	0.85 (2)	C11—H11	0.9500
N5—C7	1.3314 (18)	C12—C13	1.393 (2)
N5—C8	1.4593 (19)	C12—H12	0.9500
N5—H5N	0.91 (2)	C13—C14	1.390 (2)
C1—C4	1.4019 (18)	C13—H13	0.9500
C1—H1	0.9500	C14—C15	1.3963 (18)
C2—C3	1.3898 (19)	C14—H14	0.9500
C2—H2	0.9500	C15—H15	0.9500
C3—H3	0.9500		
C10 <sup>i</sup> —Sn1—C10	180.0	C4—C5—C6	120.21 (11)
C10 <sup>i</sup> —Sn1—N1 <sup>i</sup>	88.99 (4)	C5—C6—H6A	109.5
C10—Sn1—N1 <sup>i</sup>	91.01 (4)	C5—C6—H6B	109.5
C10 <sup>i</sup> —Sn1—N1	91.01 (4)	H6A—C6—H6B	109.5
C10—Sn1—N1	88.99 (4)	C5—C6—H6C	109.5
N1 <sup>i</sup> —Sn1—N1	180.0	H6A—C6—H6C	109.5
C10 <sup>i</sup> —Sn1—Cl1 <sup>i</sup>	89.75 (4)	H6B—C6—H6C	109.5
C10—Sn1—Cl1 <sup>i</sup>	90.25 (4)	N5—C7—N4	115.48 (12)
N1 <sup>i</sup> —Sn1—Cl1 <sup>i</sup>	91.79 (3)	N5—C7—S1	125.82 (11)
N1—Sn1—Cl1 <sup>i</sup>	88.21 (3)	N4—C7—S1	118.68 (10)
C10 <sup>i</sup> —Sn1—Cl1	90.25 (4)	N5—C8—C9	112.00 (14)
C10—Sn1—Cl1	89.75 (4)	N5—C8—H8A	109.2
N1 <sup>i</sup> —Sn1—Cl1	88.21 (3)	C9—C8—H8A	109.2
N1—Sn1—Cl1	91.79 (3)	N5—C8—H8B	109.2
Cl1 <sup>i</sup> —Sn1—Cl1	180.0	C9—C8—H8B	109.2



## supplementary materials

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C1—N1—C2	117.33 (11)	H8A—C8—H8B	107.9
C1—N1—Sn1	116.71 (9)	C8—C9—H9A	109.5
C2—N1—Sn1	125.82 (9)	C8—C9—H9B	109.5
C4—N2—C3	116.40 (12)	H9A—C9—H9B	109.5
C5—N3—N4	118.51 (11)	C8—C9—H9C	109.5
N3—N4—C7	118.86 (11)	H9A—C9—H9C	109.5
N3—N4—H4N	121.2 (14)	H9B—C9—H9C	109.5
C7—N4—H4N	118.0 (14)	C11—C10—C15	119.28 (12)
C7—N5—C8	124.90 (13)	C11—C10—Sn1	120.42 (9)
C7—N5—H5N	115.3 (14)	C15—C10—Sn1	120.29 (9)
C8—N5—H5N	119.8 (14)	C12—C11—C10	120.33 (12)
N1—C1—C4	121.53 (12)	C12—C11—H11	119.8
N1—C1—H1	119.2	C10—C11—H11	119.8
C4—C1—H1	119.2	C13—C12—C11	120.20 (13)
N1—C2—C3	120.61 (12)	C13—C12—H12	119.9
N1—C2—H2	119.7	C11—C12—H12	119.9
C3—C2—H2	119.7	C14—C13—C12	119.72 (12)
N2—C3—C2	122.68 (13)	C14—C13—H13	120.1
N2—C3—H3	118.7	C12—C13—H13	120.1
C2—C3—H3	118.7	C13—C14—C15	120.22 (12)
N2—C4—C1	121.43 (12)	C13—C14—H14	119.9
N2—C4—C5	118.35 (11)	C15—C14—H14	119.9
C1—C4—C5	120.21 (12)	C14—C15—C10	120.23 (12)
N3—C5—C4	114.09 (11)	C14—C15—H15	119.9
N3—C5—C6	125.69 (12)	C10—C15—H15	119.9
C10 <sup>i</sup> —Sn1—N1—C1	91.62 (10)	N2—C4—C5—C6	-2.00 (19)
C10—Sn1—N1—C1	-88.38 (10)	C1—C4—C5—C6	177.75 (13)
C11 <sup>i</sup> —Sn1—N1—C1	-178.66 (9)	C8—N5—C7—N4	-178.25 (14)
C11—Sn1—N1—C1	1.34 (9)	C8—N5—C7—S1	0.2 (2)
C10 <sup>i</sup> —Sn1—N1—C2	-92.92 (11)	N3—N4—C7—N5	-6.22 (18)
C10—Sn1—N1—C2	87.08 (11)	N3—N4—C7—S1	175.25 (10)
C11 <sup>i</sup> —Sn1—N1—C2	-3.20 (10)	C7—N5—C8—C9	-93.44 (18)
C11—Sn1—N1—C2	176.80 (10)	N1 <sup>i</sup> —Sn1—C10—C11	-43.26 (10)
C5—N3—N4—C7	-176.94 (12)	N1—Sn1—C10—C11	136.74 (10)
C2—N1—C1—C4	-0.57 (19)	C11 <sup>i</sup> —Sn1—C10—C11	-135.05 (10)
Sn1—N1—C1—C4	175.29 (10)	C11—Sn1—C10—C11	44.95 (10)
C1—N1—C2—C3	1.13 (19)	N1 <sup>i</sup> —Sn1—C10—C15	137.23 (10)
Sn1—N1—C2—C3	-174.31 (10)	N1—Sn1—C10—C15	-42.77 (10)
C4—N2—C3—C2	-0.6 (2)	C11 <sup>i</sup> —Sn1—C10—C15	45.44 (10)
N1—C2—C3—N2	-0.5 (2)	C11—Sn1—C10—C15	-134.56 (10)
C3—N2—C4—C1	1.20 (19)	C15—C10—C11—C12	-0.57 (19)
C3—N2—C4—C5	-179.06 (12)	Sn1—C10—C11—C12	179.92 (10)
N1—C1—C4—N2	-0.6 (2)	C10—C11—C12—C13	1.3 (2)
N1—C1—C4—C5	179.63 (12)	C11—C12—C13—C14	-0.8 (2)
N4—N3—C5—C4	179.97 (11)	C12—C13—C14—C15	-0.4 (2)
N4—N3—C5—C6	-1.2 (2)	C13—C14—C15—C10	1.1 (2)
N2—C4—C5—N3	176.87 (12)	C11—C10—C15—C14	-0.62 (19)

C1—C4—C5—N3                    -3.38 (18)  
Symmetry codes: (i)  $-x+1, -y+1, -z+1$ .

Sn1—C10—C15—C14                    178.90 (10)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N5—H5N···N3	0.91 (2)	2.16 (2)	2.6093 (17)	109.8 (16)

Fig. 1

