Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

n-Butyldichlorido{4-cyclohexyl-1-[phenyl(2-pyridyl-κN)methylene]thiosemicarbazidato-κ^2N^1,S}tin(IV) chloroform monosolvate

Md. Abu Affan,[a] Md. Abdus Salam,[a] Yang Farina[b] and Seik Weng Ng[c]*

[a]Faculty of Resource Science and Technology, Universiti Malaysia Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia, [b]School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

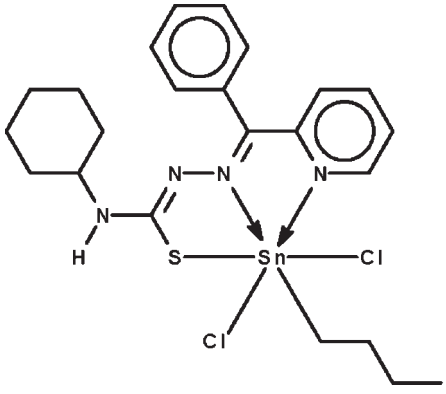
Received 19 April 2010; accepted 20 April 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; disorder in solvent or counterion; R factor = 0.058; wR factor = 0.202; data-to-parameter ratio = 21.6.

The monodeprotonated Schiff base ligand in the title compound, $[Sn(C_4H_9)(C_{19}H_{21}N_4S)Cl_2]\cdot CHCl_3$, N,N',S-chelates to the Sn atom, which is six-coordinated in an octahedral environment. The three coordinating atoms along with the butyl C atom comprise a square plane, above and below which are positioned the Cl atoms. The amino group is a hydrogen-bond donor to a Cl atom of an adjacent molecule, the hydrogen bond giving rise to a helical chain propagating in [010]. The Cl and H atoms of the chloroform molecule are disordered over two positions in an 0.67:0.33 ratio.

Related literature

For the crystal structures of other metal derivatives of the Schiff base, see: Joseph *et al.* (2004).



$CHCl_3$

Experimental

Crystal data

$[Sn(C_4H_9)(C_{19}H_{21}N_4S)Cl_2]\cdot CHCl_3$
M_r = 703.53
Monoclinic, $P2_1/n$
a = 14.5095 (9) Å
b = 13.7308 (8) Å
c = 15.7412 (10) Å
β = 94.418 (1)°
V = 3126.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.33 mm^{-1}
T = 293 K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.618, T_{max} = 0.777
29403 measured reflections
7179 independent reflections
5127 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.202
S = 1.10
7179 reflections
332 parameters
105 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C1	2.142 (7)	Sn1—S1	2.475 (2)
Sn1—N1	2.250 (5)	Sn1—Cl1	2.515 (2)
Sn1—N2	2.221 (5)	Sn1—Cl2	2.496 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···Cl1^{i}	0.86	2.54	3.383 (6)	167

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank MOSTI (grant No. 06-01-09-SF0046), Universiti Malaysia Sarawak and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5251).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Joseph, M., Suni, V., Kurup, M. R. P., Nethaji, M., Kishore, A. & Bhat, S. G. (2004). *Polyhedron*, **23**, 3069–3080.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**. Submitted.

supporting information

Acta Cryst. (2010). E**66**, m571 [https://doi.org/10.1107/S1600536810014455]

n-Butyldichlorido{4-cyclohexyl-1-[phenyl(2-pyridyl-κN)methylene]thiosemicarbazidato-κ^2N^1,S}tin(IV) chloroform monosolvate

Md. Abu Affan, Md. Abdus Salam, Yang Farina and Seik Weng Ng

S1. Comment

The mono-deprotonated anion of 2-benzoylpyridine 4-cyclohexyl thiosemicarbazone is a ligand that *N*,*N*′,*S*-binds to metal atoms (Joseph *et al.*, 2004). Whereas similar ligands have been complexed with diorganotin and triorganotin systems, the monoorganotin analogs have not been so extensively studied. The mono-deprotonated Schiff-base ligand in $SnCl_2(C_4H_9)(C_{19}H_{12}N_4S)\cdot CHCl_3$ *N*,*N*′,*S*-chelates to the tin atom, which is six-coordinate in an octahedral environment (Scheme I, Fig. 1). The three coordinating atoms along with the *ipso*-butyl carbon comprise a square plane, above and below which are positioned the chlorine atoms.

S2. Experimental

2-Benzoylpyridine 4-cyclohexyl thiosemicarbazone was synthesized by using a literature method (Joseph *et al.*, 2004). The compound (0.34 g, 1 mmol) was dissolved in dry methanol (10 ml) in a Schlenk apparatus under a nitrogen atmosphere. *n*-Butyltin trichoride (0.28 g, 1 mmol) dissolved in methanol (10 ml) was added. The mixture was heated for an hour. The solvent was removed and the yellow compound recrystallized from chloroform/methanol (1:1) in 70% yield, m.p. 478-480 K.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C—H 0.93 to 0.97, N–H 0.86 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2 to 1.5U_{eq}(C).

For the butyl chain and cyclohexyl ring, the 1,2 carbon-carbon distances were restrained to 1.54±0.01 Å and the 1,3 ones to 2.51±0.01 Å. The anisotropic displacement ellipsoids of the C_β, C_γ and C_δ atoms of the chain were restrained to be nearly isotropic.

The solvent molecule is disodered over two positions. The occupancy could not be refined, and was estimated by an examination of their temperature factors to be a 2:1 disorder. The six carbon-chlorine distances were restrained to within 0.01 Å of each other, as were the pairs of chlorine-chlorine distances. The anisotropic temperature factors were similar restrained to be nearly isotropic.

The final difference Fourier map had a peak/hole in the vicinity of the solvent molecule.

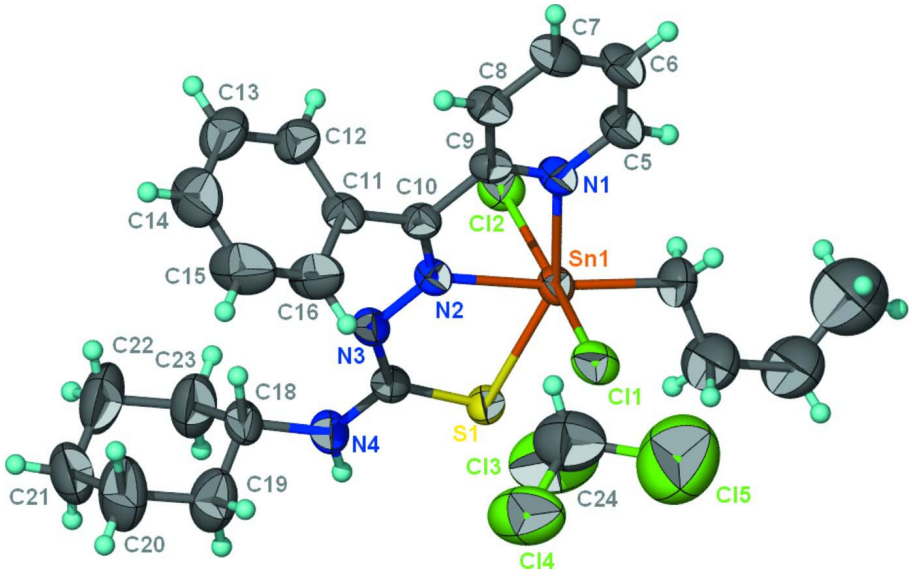


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $SnCl_2(C_4H_9)(C_{19}H_{21}N_4S)\cdot CHCl_3$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the chloroform molecule is not shown.

n-Butyldichlorido{4-cyclohexyl-1-[phenyl(2-pyridyl- κN)methylene]thiosemicarbazidato-κ^2N^1,S}tin(IV) chloroform monosolvate

Crystal data

$[Sn(C_4H_9)(C_{19}H_{21}N_4S)Cl_2]\cdot CHCl_3$
$M_r = 703.53$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 14.5095$ (9) Å
$b = 13.7308$ (8) Å
$c = 15.7412$ (10) Å
$\beta = 94.418$ (1)°
$V = 3126.8$ (3) Å^3
$Z = 4$
$F(000) = 1416$
$D_x = 1.495$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8312 reflections
$\theta = 2.3$–24.6°
$\mu = 1.33$ mm^{-1}
$T = 293$ K
Prism, orange
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.618$, $T_{max} = 0.777$
29403 measured reflections
7179 independent reflections
5127 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5$°, $\theta_{min} = 1.8$°
$h = -18\rightarrow18$
$k = -17\rightarrow17$
$l = -20\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.202$
$S = 1.10$
7179 reflections
332 parameters
105 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

$w = 1/[\sigma^2(F_o^2) + (0.1058P)^2 + 5.4806P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.48$ e Å^{-3}
$\Delta\rho_{min} = -1.14$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.64810 (3)	0.58870 (3)	0.13740 (3)	0.04946 (18)	
Cl1	0.66887 (14)	0.53556 (13)	0.29057 (11)	0.0682 (5)	
Cl2	0.65057 (13)	0.61135 (14)	−0.01975 (11)	0.0670 (4)	
Cl3	0.8024 (6)	0.4670 (4)	0.4790 (4)	0.168 (3)	0.67
Cl4	0.9050 (5)	0.3830 (5)	0.6208 (4)	0.154 (2)	0.67
Cl5	0.7217 (6)	0.3399 (7)	0.5849 (7)	0.251 (4)	0.67
Cl3′	0.7344 (11)	0.4338 (15)	0.5063 (12)	0.225 (9)	0.33
Cl4′	0.9232 (11)	0.4198 (17)	0.4959 (12)	0.282 (11)	0.33
Cl5′	0.8460 (14)	0.3630 (19)	0.6443 (6)	0.271 (13)	0.33
S1	0.70794 (10)	0.75442 (11)	0.16994 (11)	0.0531 (4)	
N1	0.6704 (4)	0.4298 (3)	0.1105 (3)	0.0500 (11)	
N2	0.7996 (3)	0.5648 (4)	0.1381 (3)	0.0458 (10)	
N3	0.8608 (3)	0.6390 (3)	0.1461 (3)	0.0518 (12)	
N4	0.8811 (4)	0.8021 (4)	0.1619 (4)	0.0697 (16)	
H4	0.8588	0.8578	0.1745	0.084*	
C1	0.5004 (5)	0.5961 (6)	0.1334 (6)	0.077 (2)	
H1A	0.4766	0.6069	0.0749	0.092*	
H1B	0.4773	0.5335	0.1509	0.092*	
C2	0.4634 (6)	0.6725 (9)	0.1871 (9)	0.133 (4)	
H2A	0.4890	0.7341	0.1702	0.159*	
H2B	0.4876	0.6604	0.2453	0.159*	
C3	0.3626 (7)	0.6855 (10)	0.1881 (10)	0.152 (5)	
H3A	0.3493	0.6944	0.2471	0.182*	
H3B	0.3470	0.7462	0.1589	0.182*	
C4	0.2979 (9)	0.6108 (13)	0.1514 (13)	0.209 (8)	
H4A	0.2355	0.6335	0.1535	0.314*	
H4B	0.3059	0.5516	0.1836	0.314*	
H4C	0.3101	0.5987	0.0933	0.314*	
C5	0.6025 (5)	0.3647 (5)	0.0968 (5)	0.0636 (17)	
H5	0.5415	0.3860	0.0928	0.076*	
C6	0.6202 (5)	0.2677 (5)	0.0883 (5)	0.0712 (19)	
H6	0.5718	0.2239	0.0774	0.085*	
C7	0.7096 (6)	0.2356 (5)	0.0961 (5)	0.0706 (19)	
H7	0.7228	0.1696	0.0914	0.085*	
C8	0.7794 (5)	0.3018 (4)	0.1109 (4)	0.0576 (15)	
H8	0.8406	0.2810	0.1172	0.069*	
C9	0.7591 (4)	0.3990 (4)	0.1165 (4)	0.0486 (13)	
C10	0.8304 (4)	0.4756 (4)	0.1303 (4)	0.0484 (13)	
C11	0.9298 (2)	0.4507 (3)	0.1343 (3)	0.0560 (15)	

C12	0.9676 (3)	0.4104 (4)	0.0638 (3)	0.0686 (18)	
H12	0.9305	0.3991	0.0140	0.082*	
C13	1.0611 (4)	0.3869 (4)	0.0678 (4)	0.088 (3)	
H13	1.0864	0.3599	0.0207	0.106*	
C14	1.1167 (3)	0.4038 (5)	0.1423 (5)	0.106 (4)	
H14	1.1792	0.3880	0.1450	0.127*	
C15	1.0788 (3)	0.4441 (6)	0.2127 (4)	0.123 (4)	
H15	1.1160	0.4554	0.2625	0.148*	
C16	0.9854 (4)	0.4676 (5)	0.2087 (3)	0.087 (3)	
H16	0.9601	0.4946	0.2559	0.105*	
C17	0.8230 (4)	0.7263 (4)	0.1580 (4)	0.0515 (13)	
C18	0.9787 (4)	0.7986 (5)	0.1466 (5)	0.072 (2)	
H18	0.9957	0.7311	0.1350	0.087*	
C19	1.0359 (5)	0.8338 (9)	0.2262 (5)	0.107 (3)	
H19A	1.0171	0.8994	0.2399	0.128*	
H19B	1.0243	0.7920	0.2739	0.128*	
C20	1.1388 (5)	0.8330 (11)	0.2126 (6)	0.136 (5)	
H20A	1.1731	0.8598	0.2626	0.163*	
H20B	1.1590	0.7663	0.2058	0.163*	
C21	1.1596 (6)	0.8913 (9)	0.1353 (7)	0.121 (5)	
H21A	1.1484	0.9597	0.1460	0.145*	
H21B	1.2245	0.8839	0.1257	0.145*	
C22	1.1017 (6)	0.8603 (10)	0.0562 (6)	0.129 (4)	
H22A	1.1201	0.7955	0.0395	0.155*	
H22B	1.1120	0.9046	0.0099	0.155*	
C23	0.9983 (5)	0.8599 (10)	0.0720 (7)	0.110 (3)	
H23A	0.9783	0.9261	0.0817	0.132*	
H23B	0.9629	0.8355	0.0216	0.132*	
C24	0.8274 (6)	0.3624 (8)	0.5359 (6)	0.134 (4)	
H24	0.8452	0.3083	0.5000	0.161*	0.67
H24′	0.8185	0.2966	0.5127	0.161*	0.33

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0436 (3)	0.0431 (3)	0.0616 (3)	−0.00057 (16)	0.00317 (18)	0.00019 (17)
Cl1	0.0875 (12)	0.0550 (9)	0.0624 (10)	−0.0180 (8)	0.0071 (8)	0.0049 (7)
Cl2	0.0722 (11)	0.0693 (10)	0.0584 (9)	−0.0024 (8)	−0.0024 (8)	0.0029 (8)
Cl3	0.247 (7)	0.095 (3)	0.162 (5)	0.047 (4)	0.004 (5)	0.012 (3)
Cl4	0.142 (4)	0.179 (5)	0.132 (4)	0.034 (4)	−0.037 (4)	−0.043 (4)
Cl5	0.218 (7)	0.239 (8)	0.300 (9)	0.027 (7)	0.053 (7)	−0.020 (7)
Cl3′	0.212 (12)	0.233 (12)	0.229 (12)	0.036 (9)	−0.001 (9)	−0.021 (9)
Cl4′	0.286 (14)	0.267 (14)	0.286 (14)	−0.009 (10)	−0.019 (10)	0.005 (10)
Cl5′	0.283 (16)	0.277 (15)	0.253 (15)	−0.022 (10)	0.017 (10)	−0.010 (10)
S1	0.0492 (8)	0.0414 (7)	0.0698 (10)	0.0030 (6)	0.0113 (7)	−0.0050 (7)
N1	0.048 (3)	0.042 (2)	0.059 (3)	−0.004 (2)	−0.003 (2)	0.000 (2)
N2	0.045 (2)	0.042 (2)	0.050 (3)	−0.0014 (19)	0.000 (2)	0.000 (2)
N3	0.046 (3)	0.037 (2)	0.073 (3)	−0.001 (2)	0.008 (2)	−0.008 (2)

N4	0.055 (3)	0.040 (3)	0.116 (5)	−0.004 (2)	0.024 (3)	−0.019 (3)
C1	0.048 (4)	0.092 (6)	0.091 (6)	0.002 (4)	0.008 (4)	−0.011 (4)
C2	0.087 (6)	0.132 (8)	0.179 (9)	0.019 (6)	0.010 (6)	−0.048 (7)
C3	0.112 (7)	0.152 (9)	0.193 (9)	0.022 (7)	0.020 (7)	−0.049 (8)
C4	0.189 (11)	0.206 (12)	0.236 (12)	0.013 (9)	0.029 (9)	−0.030 (9)
C5	0.062 (4)	0.052 (4)	0.075 (4)	−0.006 (3)	−0.002 (3)	−0.002 (3)
C6	0.070 (4)	0.055 (4)	0.087 (5)	−0.018 (3)	−0.001 (4)	−0.004 (4)
C7	0.089 (5)	0.041 (3)	0.081 (5)	−0.008 (3)	−0.001 (4)	−0.002 (3)
C8	0.066 (4)	0.039 (3)	0.067 (4)	0.002 (3)	0.000 (3)	0.001 (3)
C9	0.056 (3)	0.042 (3)	0.048 (3)	0.005 (2)	−0.001 (3)	−0.002 (2)
C10	0.049 (3)	0.040 (3)	0.055 (3)	0.005 (2)	0.001 (2)	−0.004 (2)
C11	0.053 (3)	0.039 (3)	0.075 (4)	0.004 (3)	−0.003 (3)	−0.003 (3)
C12	0.067 (4)	0.062 (4)	0.077 (5)	0.009 (3)	0.012 (4)	−0.004 (3)
C13	0.080 (6)	0.083 (5)	0.105 (7)	0.018 (4)	0.027 (5)	−0.005 (5)
C14	0.058 (5)	0.098 (7)	0.159 (11)	0.023 (5)	−0.003 (5)	−0.016 (6)
C15	0.080 (6)	0.145 (9)	0.136 (9)	0.039 (6)	−0.049 (6)	−0.053 (8)
C16	0.069 (5)	0.101 (7)	0.089 (6)	0.023 (5)	−0.017 (4)	−0.027 (5)
C17	0.052 (3)	0.041 (3)	0.062 (4)	−0.001 (2)	0.008 (3)	−0.005 (3)
C18	0.056 (4)	0.045 (3)	0.118 (6)	−0.008 (3)	0.026 (4)	−0.017 (4)
C19	0.063 (5)	0.157 (10)	0.101 (7)	0.010 (6)	0.004 (5)	0.006 (7)
C20	0.061 (6)	0.185 (14)	0.162 (11)	0.005 (7)	0.005 (6)	0.013 (11)
C21	0.075 (6)	0.105 (8)	0.186 (14)	−0.025 (5)	0.031 (8)	−0.023 (8)
C22	0.097 (8)	0.146 (11)	0.153 (11)	−0.006 (8)	0.066 (8)	0.014 (9)
C23	0.083 (6)	0.148 (10)	0.101 (7)	−0.014 (7)	0.024 (5)	0.011 (7)
C24	0.151 (8)	0.116 (7)	0.133 (8)	0.019 (7)	−0.008 (7)	−0.009 (7)

Geometric parameters (Å, º)

Sn1—C1	2.142 (7)	C7—C8	1.368 (9)
Sn1—N1	2.250 (5)	C7—H7	0.9300
Sn1—N2	2.221 (5)	C8—C9	1.371 (8)
Sn1—S1	2.475 (2)	C8—H8	0.9300
Sn1—Cl1	2.515 (2)	C9—C10	1.479 (8)
Sn1—Cl2	2.496 (2)	C10—C11	1.480 (7)
Cl3—C24	1.715 (8)	C11—C12	1.3900
Cl4—C24	1.704 (8)	C11—C16	1.3900
Cl5—C24	1.795 (8)	C12—C13	1.3900
Cl3′—C24	1.703 (10)	C12—H12	0.9300
Cl4′—C24	1.755 (9)	C13—C14	1.3900
Cl5′—C24	1.707 (10)	C13—H13	0.9300
S1—C17	1.738 (6)	C14—C15	1.3900
N1—C5	1.336 (8)	C14—H14	0.9300
N1—C9	1.350 (8)	C15—C16	1.3900
N2—C10	1.313 (7)	C15—H15	0.9300
N2—N3	1.351 (7)	C16—H16	0.9300
N3—C17	1.338 (7)	C18—C23	1.489 (12)
N4—C17	1.337 (8)	C18—C19	1.527 (8)
N4—C18	1.456 (8)	C18—H18	0.9800

N4—H4	0.8600	C19—C20	1.525 (8)
C1—C2	1.474 (8)	C19—H19A	0.9700
C1—H1A	0.9700	C19—H19B	0.9700
C1—H1B	0.9700	C20—C21	1.507 (9)
C2—C3	1.475 (8)	C20—H20A	0.9700
C2—H2A	0.9700	C20—H20B	0.9700
C2—H2B	0.9700	C21—C22	1.510 (9)
C3—C4	1.478 (9)	C21—H21A	0.9700
C3—H3A	0.9700	C21—H21B	0.9700
C3—H3B	0.9700	C22—C23	1.540 (8)
C4—H4A	0.9600	C22—H22A	0.9700
C4—H4B	0.9600	C22—H22B	0.9700
C4—H4C	0.9600	C23—H23A	0.9700
C5—C6	1.364 (10)	C23—H23B	0.9700
C5—H5	0.9300	C24—H24	0.9800
C6—C7	1.367 (11)	C24—H24′	0.9801
C6—H6	0.9300		

C1—Sn1—N2	174.1 (2)	C15—C14—C13	120.0
C1—Sn1—N1	101.4 (2)	C15—C14—H14	120.0
N2—Sn1—N1	72.61 (18)	C13—C14—H14	120.0
C1—Sn1—S1	107.3 (2)	C14—C15—C16	120.0
N2—Sn1—S1	78.67 (13)	C14—C15—H15	120.0
N1—Sn1—S1	151.28 (13)	C16—C15—H15	120.0
C1—Sn1—Cl2	93.2 (2)	C15—C16—C11	120.0
N2—Sn1—Cl2	86.17 (13)	C15—C16—H16	120.0
N1—Sn1—Cl2	85.49 (14)	C11—C16—H16	120.0
S1—Sn1—Cl2	93.38 (6)	N4—C17—N3	116.1 (5)
C1—Sn1—Cl1	95.0 (3)	N4—C17—S1	115.5 (4)
N2—Sn1—Cl1	84.68 (13)	N3—C17—S1	128.4 (5)
N1—Sn1—Cl1	83.71 (14)	N4—C18—C23	111.0 (6)
S1—Sn1—Cl1	93.11 (6)	N4—C18—C19	109.1 (6)
Cl2—Sn1—Cl1	167.54 (7)	C23—C18—C19	110.1 (7)
C17—S1—Sn1	95.6 (2)	N4—C18—H18	108.9
C5—N1—C9	119.3 (5)	C23—C18—H18	108.9
C5—N1—Sn1	124.4 (5)	C19—C18—H18	108.9
C9—N1—Sn1	116.1 (4)	C20—C19—C18	111.0 (6)
C10—N2—N3	119.1 (5)	C20—C19—H19A	109.4
C10—N2—Sn1	118.7 (4)	C18—C19—H19A	109.4
N3—N2—Sn1	122.2 (4)	C20—C19—H19B	109.4
C17—N3—N2	114.5 (5)	C18—C19—H19B	109.4
C17—N4—C18	125.8 (5)	H19A—C19—H19B	108.0
C17—N4—H4	117.1	C21—C20—C19	111.6 (7)
C18—N4—H4	117.1	C21—C20—H20A	109.3
C2—C1—Sn1	115.1 (6)	C19—C20—H20A	109.3
C2—C1—H1A	108.5	C21—C20—H20B	109.3
Sn1—C1—H1A	108.5	C19—C20—H20B	109.3
C2—C1—H1B	108.5	H20A—C20—H20B	108.0

Sn1—C1—H1B	108.5	C22—C21—C20	112.5 (7)
H1A—C1—H1B	107.5	C22—C21—H21A	109.1
C1—C2—C3	119.8 (7)	C20—C21—H21A	109.1
C1—C2—H2A	107.4	C22—C21—H21B	109.1
C3—C2—H2A	107.4	C20—C21—H21B	109.1
C1—C2—H2B	107.4	H21A—C21—H21B	107.8
C3—C2—H2B	107.4	C21—C22—C23	110.8 (7)
H2A—C2—H2B	106.9	C21—C22—H22A	109.5
C4—C3—C2	120.8 (9)	C23—C22—H22A	109.5
C4—C3—H3A	107.1	C21—C22—H22B	109.5
C2—C3—H3A	107.1	C23—C22—H22B	109.5
C4—C3—H3B	107.1	H22A—C22—H22B	108.1
C2—C3—H3B	107.1	C18—C23—C22	112.1 (8)
H3A—C3—H3B	106.8	C18—C23—H23A	109.2
C3—C4—H4A	109.5	C22—C23—H23A	109.2
C3—C4—H4B	109.5	C18—C23—H23B	109.2
H4A—C4—H4B	109.5	C22—C23—H23B	109.2
C3—C4—H4C	109.5	H23A—C23—H23B	107.9
H4A—C4—H4C	109.5	Cl5′—C24—Cl4	34.0 (7)
H4B—C4—H4C	109.5	Cl5′—C24—Cl3′	109.4 (8)
N1—C5—C6	121.8 (7)	Cl4—C24—Cl3′	125.5 (11)
N1—C5—H5	119.1	Cl5′—C24—Cl3	121.9 (12)
C6—C5—H5	119.1	Cl4—C24—Cl3	111.8 (7)
C7—C6—C5	119.3 (7)	Cl3′—C24—Cl3	41.0 (7)
C7—C6—H6	120.3	Cl5′—C24—Cl4′	106.7 (7)
C5—C6—H6	120.3	Cl4—C24—Cl4′	73.3 (7)
C6—C7—C8	119.1 (6)	Cl3′—C24—Cl4′	106.0 (7)
C6—C7—H7	120.4	Cl3—C24—Cl4′	65.1 (7)
C8—C7—H7	120.4	Cl5′—C24—Cl5	69.3 (7)
C9—C8—C7	119.8 (7)	Cl4—C24—Cl5	103.1 (6)
C9—C8—H8	120.1	Cl3′—C24—Cl5	62.1 (7)
C7—C8—H8	120.1	Cl3—C24—Cl5	102.5 (6)
N1—C9—C8	120.6 (6)	Cl4′—C24—Cl5	163.2 (12)
N1—C9—C10	116.1 (5)	Cl5′—C24—H24	123.4
C8—C9—C10	123.3 (6)	Cl4—C24—H24	112.9
N2—C10—C11	123.3 (5)	Cl3′—C24—H24	121.2
N2—C10—C9	116.0 (5)	Cl3—C24—H24	112.9
C11—C10—C9	120.7 (5)	Cl4′—C24—H24	83.2
C12—C11—C16	120.0	Cl5—C24—H24	112.9
C12—C11—C10	120.1 (4)	Cl5′—C24—H24′	112.5
C16—C11—C10	119.9 (4)	Cl4—C24—H24′	120.3
C13—C12—C11	120.0	Cl3′—C24—H24′	110.5
C13—C12—H12	120.0	Cl3—C24—H24′	124.2
C11—C12—H12	120.0	Cl4′—C24—H24′	111.5
C12—C13—C14	120.0	Cl5—C24—H24′	84.7
C12—C13—H13	120.0	H24—C24—H24′	28.2
C14—C13—H13	120.0		

C1—Sn1—S1—C17	−174.4 (3)	C5—N1—C9—C10	179.0 (6)
N2—Sn1—S1—C17	5.4 (2)	Sn1—N1—C9—C10	−6.7 (7)
N1—Sn1—S1—C17	6.8 (4)	C7—C8—C9—N1	2.3 (10)
Cl2—Sn1—S1—C17	−80.0 (2)	C7—C8—C9—C10	−178.5 (6)
Cl1—Sn1—S1—C17	89.4 (2)	N3—N2—C10—C11	3.3 (9)
C1—Sn1—N1—C5	0.0 (6)	Sn1—N2—C10—C11	−176.8 (4)
N2—Sn1—N1—C5	−179.7 (6)	N3—N2—C10—C9	−176.4 (5)
S1—Sn1—N1—C5	178.9 (4)	Sn1—N2—C10—C9	3.5 (7)
Cl2—Sn1—N1—C5	−92.3 (5)	N1—C9—C10—N2	2.2 (8)
Cl1—Sn1—N1—C5	93.9 (5)	C8—C9—C10—N2	−177.0 (6)
C1—Sn1—N1—C9	−174.0 (5)	N1—C9—C10—C11	−177.5 (5)
N2—Sn1—N1—C9	6.2 (4)	C8—C9—C10—C11	3.3 (9)
S1—Sn1—N1—C9	4.8 (6)	N2—C10—C11—C12	−117.1 (6)
Cl2—Sn1—N1—C9	93.6 (4)	C9—C10—C11—C12	62.6 (7)
Cl1—Sn1—N1—C9	−80.1 (4)	N2—C10—C11—C16	63.1 (7)
C1—Sn1—N2—C10	−8 (3)	C9—C10—C11—C16	−117.3 (5)
N1—Sn1—N2—C10	−5.2 (4)	C16—C11—C12—C13	0.0
S1—Sn1—N2—C10	174.1 (5)	C10—C11—C12—C13	−179.8 (5)
Cl2—Sn1—N2—C10	−91.7 (4)	C11—C12—C13—C14	0.0
Cl1—Sn1—N2—C10	79.9 (4)	C12—C13—C14—C15	0.0
C1—Sn1—N2—N3	172 (2)	C13—C14—C15—C16	0.0
N1—Sn1—N2—N3	174.7 (5)	C14—C15—C16—C11	0.0
S1—Sn1—N2—N3	−6.0 (4)	C12—C11—C16—C15	0.0
Cl2—Sn1—N2—N3	88.3 (4)	C10—C11—C16—C15	179.8 (5)
Cl1—Sn1—N2—N3	−100.2 (4)	C18—N4—C17—N3	6.0 (11)
C10—N2—N3—C17	−176.7 (6)	C18—N4—C17—S1	−174.4 (6)
Sn1—N2—N3—C17	3.4 (7)	N2—N3—C17—N4	−176.7 (6)
N2—Sn1—C1—C2	154 (2)	N2—N3—C17—S1	3.7 (9)
N1—Sn1—C1—C2	151.1 (9)	Sn1—S1—C17—N4	173.2 (5)
S1—Sn1—C1—C2	−28.3 (9)	Sn1—S1—C17—N3	−7.3 (6)
Cl2—Sn1—C1—C2	−122.8 (9)	C17—N4—C18—C23	117.7 (9)
Cl1—Sn1—C1—C2	66.6 (9)	C17—N4—C18—C19	−120.8 (9)
Sn1—C1—C2—C3	178.8 (11)	N4—C18—C19—C20	−179.1 (8)
C1—C2—C3—C4	13 (3)	C23—C18—C19—C20	−57.1 (11)
C9—N1—C5—C6	−0.2 (11)	C18—C19—C20—C21	55.1 (13)
Sn1—N1—C5—C6	−174.0 (6)	C19—C20—C21—C22	−53.4 (14)
N1—C5—C6—C7	1.6 (12)	C20—C21—C22—C23	52.4 (14)
C5—C6—C7—C8	−1.0 (12)	N4—C18—C23—C22	178.1 (8)
C6—C7—C8—C9	−0.9 (11)	C19—C18—C23—C22	57.2 (11)
C5—N1—C9—C8	−1.8 (9)	C21—C22—C23—C18	−55.0 (13)
Sn1—N1—C9—C8	172.6 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···Cl1^{i}	0.86	2.54	3.383 (6)	167

Symmetry code: (i) −*x*+3/2, *y*+1/2, −*z*+1/2.