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Chlorodiethyl[4-(4-nitrophenyl)piperazine-1-carbodithioato]tin(IV)

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Key indicators

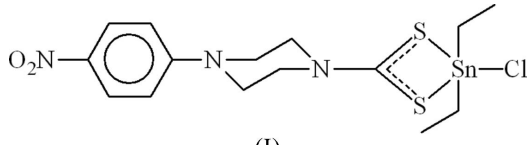
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.062
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $[Sn(C_2H_5)_2(C_{11}H_{12}N_3O_2S_2)Cl]$, features an asymmetrically chelating thiocarboxylate ligand. The Sn atom is five-coordinate within a C_2ClS_2 donor set that is best described as trigonal bipyramidal with S and Cl atoms in axial positions, defining a bond angle of 156.58 (2)°.

Comment

Complexing agents with a dithio functional group have been widely used in industry as rodent repellents, vulcanization additives in the manufacture of rubber, additives in lubricants and in agriculture as fungicides on almond trees, stone fruits and vegetables.



(I)

As in a similar compound in the literature (Stiefel & Matsumoto, 1995), the Sn atom is five-coordinate. The geometry of the complex (I) is approximately trigonal bipyramidal, with atoms C12, S1 and C14 occupying the equatorial positions. The sum of the equatorial angles (359.27°) at the tin atom involving the two coordinated C atoms and one S atom [S1—Sn—C12 = 119.25 (6)°, S1—Sn—C14 = 116.36 (7)° and C12—Sn—C14 = 123.66 (9)°] deviates by only 0.73° from 360°, so atoms C12, S1, C14 and Sn are approximately coplanar; the Sn atom is displaced by 0.111 (1) Å from the least-squares plane formed by S1, C12 and C14, and is on the same side as Cl.

The Cl atom occupies approximately one axial position of the trigonal bipyramid; the angle between the Sn—Cl bond and the equatorial plane is 83.66 (9)°. Conversely, because of

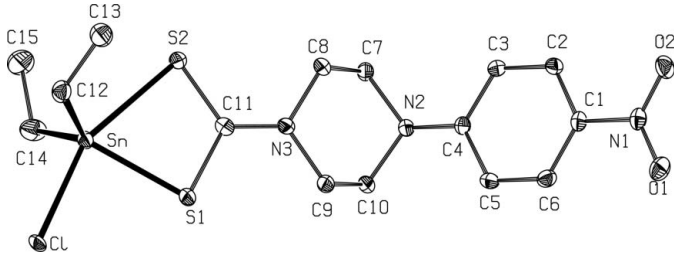


Figure 1
The molecular structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms have been omitted for clarity.

the constraint of the chelate [the S1—Sn—S2 angle is only 69.59 (2)°, the angle between the Sn—S2 bond and the equatorial plane is 72.10 (9)°]; atom S2 cannot exactly occupy the second *trans* axial position of the trigonal bipyramid, the angle Cl—Sn—S2 being 156.58 (2)°.

The S—C bond lengths [S1—C11 = 1.752 (3) Å and S2—C11 = 1.716 (2) Å] appear to be characteristic of the thiocarboxylate group and these distances are all intermediate between the values expected for single and double bonds (Tiekink, 1992).

Experimental

To a solution of 4-(4-nitrophenyl)piperazine-1-carbodithioic acid (0.3 g, 1.059 mmol) in dry methanol (50 ml) was added diethyltin(IV) chloride (0.262 g, 1.059 mmol), dissolved in methanol (30 ml), dropwise and the mixture was stirred vigorously for 3 h. The resulting yellow solid was separated and the filtrate was allowed to evaporate, yielding yellow crystals.

Crystal data

$[Sn(C_2H_5)_2(C_{11}H_{12}N_3O_2S_2)Cl]$	$Z = 4$
$M_r = 494.65$	$D_x = 1.735$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.1638$ (9) Å	$\mu = 1.73$ mm^{-1}
$b = 10.5851$ (7) Å	$T = 100$ (1) K
$c = 14.0247$ (9) Å	Trianglar block, yellow
$\beta = 115.799$ (1)°	0.49 × 0.42 × 0.35 mm
$V = 1893.1$ (2) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	16982 measured reflections
	4661 independent reflections
φ and ω scans	4332 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	$R_{int} = 0.021$
	$\theta_{max} = 28.3°$
$T_{min} = 0.430$, $T_{max} = 0.549$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 2.2398P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.024$	
$wR(F^2) = 0.062$	
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
4661 reflections	$\Delta\rho_{max} = 1.25$ e Å^{-3}
305 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
All H-atom parameters refined	

The final difference Fourier map was essentially featureless, except for one peak of 1.25 (9) e Å^{-3} within 1.0 Å of Cl. All H atoms were freely refined, with C—H = 0.87 (3)–1.01 (4) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2000); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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supporting information

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Crystal data

$[Sn(C_2H_5)_2(C_{11}H_{12}N_3O_2S_2)Cl]$
$M_r = 494.65$
Monoclinic, $P2_1/c$
Hall symbol: -P 2y b c
$a = 14.1638\ (9)$ Å
$b = 10.5851\ (7)$ Å
$c = 14.0247\ (9)$ Å
$\beta = 115.799\ (1)°$
$V = 1893.1\ (2)$ Å^3
$Z = 4$
$F(000) = 992$

The final unit cell was obtained from the xyz centroids of 5242 reflections after integration using the SAINTPLUS software package (Bruker, 2000).
Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the finalatomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
$D_x = 1.735$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5242 reflections
$\theta = 2.5–29.6°$
$\mu = 1.73$ mm^{-1}
$T = 100$ K
Trianglar block, yellow
0.49 × 0.42 × 0.35 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine focus sealed Siemens Mo tube
Parallel mounted graphite monochromator
Detector resolution: 4096x4096 / 62x62 (binned 512) pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

$T_{min} = 0.430$, $T_{max} = 0.549$
16982 measured reflections
4661 independent reflections
4332 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.5°$
$h = -18\rightarrow16$
$k = -14\rightarrow14$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.062$
$S = 1.07$
4661 reflections
305 parameters
0 restraints
Primary atom site location: heavy-atom method

Secondary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 2.2398P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn	0.06969 (1)	0.23293 (1)	0.29408 (1)	0.0143 (1)
Cl	−0.11109 (4)	0.19507 (5)	0.28215 (4)	0.0170 (1)
S1	0.08452 (4)	0.41066 (5)	0.41456 (4)	0.0168 (2)
S2	0.25528 (4)	0.35152 (5)	0.35415 (4)	0.0168 (2)
O1	0.36114 (14)	1.29089 (15)	0.64523 (14)	0.0231 (5)
O2	0.48872 (14)	1.27462 (15)	0.59962 (14)	0.0224 (5)
N1	0.42322 (16)	1.22714 (17)	0.62536 (14)	0.0168 (5)
N2	0.40698 (14)	0.69539 (17)	0.64976 (14)	0.0135 (5)
N3	0.26164 (14)	0.54391 (17)	0.48052 (14)	0.0142 (5)
C1	0.41949 (17)	1.09049 (19)	0.63219 (16)	0.0146 (5)
C2	0.49031 (17)	1.0166 (2)	0.61263 (16)	0.0150 (6)
C3	0.48520 (17)	0.8863 (2)	0.61714 (17)	0.0149 (6)
C4	0.40907 (16)	0.82616 (19)	0.64143 (15)	0.0127 (5)
C5	0.33951 (17)	0.9046 (2)	0.66236 (17)	0.0162 (6)
C6	0.34489 (17)	1.0344 (2)	0.65790 (17)	0.0165 (6)
C7	0.44451 (17)	0.6135 (2)	0.58890 (17)	0.0152 (6)
C8	0.35810 (17)	0.5924 (2)	0.47702 (17)	0.0166 (6)
C9	0.22677 (17)	0.6194 (2)	0.54797 (17)	0.0154 (6)
C10	0.31822 (17)	0.6341 (2)	0.65770 (16)	0.0144 (6)
C11	0.20862 (16)	0.4468 (2)	0.42303 (16)	0.0144 (6)
C12	0.0106 (2)	0.2682 (2)	0.12730 (19)	0.0205 (6)
C13	0.0752 (2)	0.3504 (3)	0.08976 (19)	0.0250 (7)
C14	0.1402 (2)	0.0587 (3)	0.3675 (2)	0.0274 (8)
C15	0.2238 (3)	0.0120 (3)	0.3377 (3)	0.0360 (10)
H2	0.540 (2)	1.056 (3)	0.596 (2)	0.019 (7)*
H3	0.533 (2)	0.842 (3)	0.608 (2)	0.015 (6)*
H5	0.289 (2)	0.874 (3)	0.677 (2)	0.027 (8)*
H6	0.302 (2)	1.083 (3)	0.670 (2)	0.015 (6)*
H7	0.4639 (19)	0.536 (2)	0.6239 (19)	0.011 (6)*
H7′	0.508 (2)	0.647 (3)	0.586 (2)	0.025 (7)*
H8	0.341 (2)	0.669 (3)	0.439 (2)	0.016 (6)*
H8′	0.378 (2)	0.534 (3)	0.438 (2)	0.023 (7)*
H9	0.171 (2)	0.580 (2)	0.555 (2)	0.015 (6)*
H9′	0.208 (2)	0.705 (3)	0.516 (2)	0.018 (7)*
H10	0.297 (2)	0.681 (3)	0.704 (2)	0.019 (7)*
H10′	0.344 (2)	0.549 (3)	0.689 (2)	0.015 (6)*

H12	0.008 (2)	0.184 (3)	0.101 (2)	0.027 (7)*
H12′	−0.061 (3)	0.303 (3)	0.111 (2)	0.032 (8)*
H13	0.089 (2)	0.436 (3)	0.123 (2)	0.030 (8)*
H13′	0.139 (2)	0.306 (3)	0.099 (2)	0.026 (7)*
H13"	0.034 (2)	0.365 (3)	0.012 (2)	0.028 (8)*
H14	0.157 (3)	0.067 (4)	0.436 (3)	0.051 (11)*
H14′	0.089 (4)	0.002 (4)	0.347 (4)	0.080 (15)*
H15	0.193 (4)	0.002 (4)	0.263 (4)	0.080 (15)*
H15′	0.251 (3)	−0.068 (4)	0.368 (3)	0.058 (11)*
H15"	0.273 (3)	0.076 (4)	0.351 (3)	0.059 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.0125 (1)	0.0134 (1)	0.0166 (1)	−0.0018 (1)	0.0060 (1)	−0.0014 (1)
Cl	0.0100 (2)	0.0165 (2)	0.0264 (3)	−0.0034 (2)	0.0096 (2)	−0.0030 (2)
S1	0.0134 (3)	0.0156 (3)	0.0229 (3)	−0.0031 (2)	0.0092 (2)	−0.0043 (2)
S2	0.0145 (3)	0.0196 (3)	0.0177 (2)	−0.0043 (2)	0.0083 (2)	−0.0057 (2)
O1	0.0277 (9)	0.0153 (8)	0.0267 (9)	0.0041 (7)	0.0121 (8)	−0.0005 (6)
O2	0.0290 (10)	0.0164 (8)	0.0240 (8)	−0.0055 (7)	0.0135 (7)	0.0008 (6)
N1	0.0210 (10)	0.0122 (9)	0.0147 (8)	−0.0010 (7)	0.0055 (8)	−0.0002 (7)
N2	0.0134 (9)	0.0120 (8)	0.0154 (8)	−0.0012 (6)	0.0067 (7)	−0.0012 (6)
N3	0.0123 (8)	0.0163 (9)	0.0147 (8)	−0.0021 (7)	0.0065 (7)	−0.0016 (7)
C1	0.0172 (10)	0.0116 (9)	0.0135 (9)	−0.0006 (8)	0.0053 (8)	−0.0006 (7)
C2	0.0159 (10)	0.0166 (10)	0.0143 (9)	−0.0025 (8)	0.0082 (8)	−0.0011 (7)
C3	0.0141 (10)	0.0155 (10)	0.0168 (9)	0.0005 (8)	0.0084 (8)	−0.0014 (8)
C4	0.0125 (10)	0.0123 (9)	0.0114 (9)	−0.0001 (7)	0.0035 (8)	−0.0002 (7)
C5	0.0152 (10)	0.0170 (10)	0.0196 (10)	−0.0006 (8)	0.0107 (9)	−0.0001 (8)
C6	0.0157 (10)	0.0170 (10)	0.0183 (10)	0.0021 (8)	0.0088 (9)	−0.0011 (8)
C7	0.0115 (10)	0.0133 (10)	0.0200 (10)	0.0000 (8)	0.0060 (8)	−0.0028 (8)
C8	0.0153 (10)	0.0173 (10)	0.0189 (10)	−0.0048 (8)	0.0091 (9)	−0.0034 (8)
C9	0.0122 (10)	0.0156 (10)	0.0185 (10)	−0.0012 (8)	0.0067 (8)	−0.0028 (8)
C10	0.0149 (10)	0.0140 (10)	0.0155 (9)	−0.0030 (8)	0.0077 (8)	−0.0009 (7)
C11	0.0124 (10)	0.0165 (10)	0.0129 (9)	−0.0001 (8)	0.0043 (8)	0.0026 (7)
C12	0.0196 (12)	0.0204 (11)	0.0194 (10)	−0.0023 (9)	0.0065 (9)	−0.0036 (9)
C13	0.0273 (13)	0.0284 (13)	0.0189 (11)	−0.0049 (10)	0.0096 (10)	−0.0021 (9)
C14	0.0281 (14)	0.0227 (12)	0.0379 (14)	0.0073 (10)	0.0204 (12)	0.0082 (10)
C15	0.0340 (16)	0.0243 (14)	0.058 (2)	0.0075 (12)	0.0278 (15)	−0.0017 (13)

Geometric parameters (Å, º)

Sn—Cl	2.5243 (7)	C12—C13	1.514 (4)
Sn—S1	2.4758 (6)	C14—C15	1.501 (5)
Sn—S2	2.6959 (6)	C2—H2	0.93 (3)
Sn—C12	2.146 (2)	C3—H3	0.88 (3)
Sn—C14	2.136 (3)	C5—H5	0.89 (3)
S1—C11	1.752 (3)	C6—H6	0.87 (3)
S2—C11	1.716 (2)	C7—H7	0.93 (2)

O1—N1	1.233 (3)	C7—H7′	0.98 (3)
O2—N1	1.239 (3)	C8—H8	0.94 (3)
N1—C1	1.452 (3)	C8—H8′	0.95 (3)
N2—C4	1.391 (3)	C9—H9	0.94 (3)
N2—C7	1.469 (3)	C9—H9′	0.99 (3)
N2—C10	1.461 (3)	C10—H10	0.96 (3)
N3—C8	1.480 (3)	C10—H10′	1.00 (3)
N3—C9	1.478 (3)	C12—H12	0.96 (3)
N3—C11	1.321 (3)	C12—H12′	1.01 (4)
C1—C2	1.390 (3)	C13—H13	1.00 (3)
C1—C6	1.390 (4)	C13—H13′	0.98 (3)
C2—C3	1.384 (3)	C13—H13"	1.00 (3)
C3—C4	1.416 (3)	C14—H14	0.89 (4)
C4—C5	1.414 (3)	C14—H14′	0.89 (5)
C5—C6	1.379 (3)	C15—H15	0.95 (5)
C7—C8	1.529 (3)	C15—H15′	0.95 (4)
C9—C10	1.528 (3)	C15—H15"	0.93 (5)
Sn···H14′^{i}	3.63 (5)	C2···H2^{ix}	2.87 (3)
Sn···H13"^{ii}	3.47 (3)	C3···H2^{ix}	2.92 (3)
Cl···S1	3.4430 (8)	C3···H7′	2.61 (3)
Cl···C12	3.398 (3)	C4···H9′	2.91 (3)
Cl···C14	3.532 (3)	C4···H8	3.06 (3)
Cl···H12′	3.01 (3)	C5···H10	2.57 (3)
Cl···H13^{iii}	3.00 (3)	C5···H9′	2.97 (3)
Cl···H5^{iv}	2.91 (3)	C6···H7^{viii}	3.08 (3)
Cl···H10^{iv}	3.02 (3)	C7···H3	2.68 (3)
Cl···H13"^{ii}	3.04 (3)	C8···H10′	3.10 (3)
S1···Cl	3.4430 (8)	C10···H5	2.61 (3)
S1···S2	2.9569 (9)	C12···H9′^{iii}	2.94 (3)
S2···C12	3.649 (3)	C12···H14′^{i}	2.95 (5)
S2···C13	3.467 (3)	C13···H14^{xiii}	2.99 (4)
S2···S1	2.9569 (9)	C13···H6^{v}	2.99 (3)
S2···C15	3.616 (3)	C14···H12′^{iii}	3.00 (3)
S2···C14	3.545 (3)	H2···O2	2.43 (3)
S2···C6^{v}	3.699 (2)	H2···C2^{ix}	2.87 (3)
S1···H12^{i}	3.14 (3)	H2···C3^{ix}	2.92 (3)
S1···H9	2.55 (2)	H3···C7	2.68 (3)
S2···H8′	2.52 (3)	H3···H7′	2.09 (4)
S2···H15"	2.93 (4)	H5···C10	2.61 (3)
S2···H7′^{vi}	3.08 (3)	H5···H10	2.07 (4)
S2···H13	3.20 (3)	H5···Cl^{iv}	2.91 (3)
S2···H6^{v}	3.01 (3)	H6···O1	2.43 (3)
O1···C11^{vii}	3.353 (3)	H6···S2^{xi}	3.01 (3)
O1···C4^{viii}	3.348 (3)	H6···C13^{xi}	2.99 (3)
O1···C3^{viii}	3.248 (3)	H6···H13′^{xi}	2.39 (4)
O2···C8^{ix}	3.142 (3)	H7···O2^{xii}	2.83 (2)
O2···C7^{ix}	3.386 (3)	H7···H10′	2.26 (4)

O2···C4^{viii}	3.318 (3)	H7···C6^{x}	3.08 (3)
O1···H6	2.43 (3)	H7′···C3	2.61 (3)
O1···H10′^{vii}	2.83 (3)	H7′···H3	2.09 (4)
O2···H2	2.43 (3)	H7′···S2^{vi}	3.08 (3)
O2···H7^{vii}	2.83 (2)	H7′···O2^{ix}	2.75 (3)
O2···H7′^{ix}	2.75 (3)	H8···C4	3.06 (3)
O2···H8^{ix}	2.76 (3)	H8···H9′	2.58 (4)
N1···N2^{viii}	3.040 (3)	H8···O2^{ix}	2.76 (3)
N1···C4^{viii}	3.267 (3)	H8′···S2	2.52 (3)
N2···N3	2.862 (3)	H9···S1	2.55 (2)
N2···N1^{x}	3.040 (3)	H9′···C4	2.91 (3)
N2···C1^{x}	3.175 (3)	H9′···C5	2.97 (3)
N3···N2	2.862 (3)	H9′···H8	2.58 (4)
C1···N2^{viii}	3.175 (3)	H9′···C12^{i}	2.94 (3)
C1···C7^{viii}	3.537 (3)	H9′···H12′^{i}	2.31 (4)
C2···C10^{viii}	3.417 (3)	H10···C5	2.57 (3)
C2···C2^{ix}	3.307 (3)	H10···H5	2.07 (4)
C2···C3^{ix}	3.540 (3)	H10···Cl^{iv}	3.02 (3)
C3···C2^{ix}	3.540 (3)	H10′···O1^{xii}	2.83 (3)
C3···O1^{x}	3.248 (3)	H10′···C8	3.10 (3)
C4···O1^{x}	3.348 (3)	H10′···H7	2.26 (4)
C4···O2^{x}	3.318 (3)	H10′···C2^{x}	2.77 (3)
C4···N1^{x}	3.267 (3)	H12···S1^{iii}	3.14 (3)
C5···C9	3.465 (3)	H12′···C14^{i}	3.00 (3)
C6···S2^{xi}	3.699 (2)	H12′···H9′^{iii}	2.31 (4)
C7···C1^{x}	3.537 (3)	H12′···H14′^{i}	2.27 (6)
C7···O2^{ix}	3.386 (3)	H13···S2	3.20 (3)
C8···O2^{ix}	3.142 (3)	H13···Cl^{i}	3.00 (3)
C9···C12^{i}	3.554 (4)	H13′···H6^{v}	2.39 (4)
C9···C5	3.465 (3)	H13"···Sn^{xiii}	3.47 (3)
C10···C2^{x}	3.417 (3)	H13"···Cl^{xiii}	3.04 (3)
C11···O1^{xii}	3.353 (3)	H13"···H14^{xiii}	2.51 (5)
C12···C9^{iii}	3.554 (4)	H14···C13^{ii}	2.99 (4)
C12···S2	3.649 (3)	H14···H13"^{ii}	2.51 (5)
C12···Cl	3.398 (3)	H14′···Sn^{iii}	3.63 (5)
C14···S2	3.545 (3)	H14′···C12^{iii}	2.95 (5)
C14···Cl	3.532 (3)	H14′···H12′^{iii}	2.27 (6)
C2···H10′^{viii}	2.77 (3)	H15"···S2	2.93 (4)

Cl—Sn—S1	87.03 (2)	C6—C5—H5	116 (2)
Cl—Sn—S2	156.58 (2)	C1—C6—H6	118 (2)
Cl—Sn—C12	92.99 (8)	C5—C6—H6	122 (2)
Cl—Sn—C14	98.21 (8)	N2—C7—H7	108.1 (16)
S1—Sn—S2	69.59 (2)	N2—C7—H7′	112.3 (17)
S1—Sn—C12	119.25 (6)	C8—C7—H7	109.4 (15)
S1—Sn—C14	116.36 (7)	C8—C7—H7′	110.4 (15)
S2—Sn—C12	97.14 (8)	H7—C7—H7′	106 (3)
S2—Sn—C14	93.65 (8)	N3—C8—H8	107.7 (19)

C12—Sn—C14	123.66 (9)	N3—C8—H8′	107.7 (19)
Sn—S1—C11	89.82 (7)	C7—C8—H8	110.4 (17)
Sn—S2—C11	83.54 (8)	C7—C8—H8′	112.5 (17)
O1—N1—O2	122.82 (19)	H8—C8—H8′	108 (2)
O1—N1—C1	118.7 (2)	N3—C9—H9	111.1 (15)
O2—N1—C1	118.5 (2)	N3—C9—H9′	107.6 (16)
C4—N2—C7	120.82 (19)	C10—C9—H9	108.9 (16)
C4—N2—C10	119.9 (2)	C10—C9—H9′	107.7 (16)
C7—N2—C10	108.86 (17)	H9—C9—H9′	112 (2)
C8—N3—C9	113.84 (17)	N2—C10—H10	110.7 (19)
C8—N3—C11	122.52 (19)	N2—C10—H10′	105.8 (18)
C9—N3—C11	123.5 (2)	C9—C10—H10	110.8 (17)
N1—C1—C2	119.8 (2)	C9—C10—H10′	109.8 (16)
N1—C1—C6	119.8 (2)	H10—C10—H10′	109 (2)
C2—C1—C6	120.42 (19)	Sn—C12—H12	100.9 (16)
C1—C2—C3	119.7 (2)	Sn—C12—H12′	100.8 (16)
C2—C3—C4	121.3 (2)	C13—C12—H12	109.2 (18)
N2—C4—C3	120.9 (2)	C13—C12—H12′	114.3 (19)
N2—C4—C5	121.7 (2)	H12—C12—H12′	113 (3)
C3—C4—C5	117.30 (19)	C12—C13—H13	112.6 (17)
C4—C5—C6	121.2 (2)	C12—C13—H13′	110.0 (18)
C1—C6—C5	120.1 (2)	C12—C13—H13"	108.3 (18)
N2—C7—C8	110.6 (2)	H13—C13—H13′	113 (3)
N3—C8—C7	110.78 (18)	H13—C13—H13"	106 (2)
N3—C9—C10	109.1 (2)	H13′—C13—H13"	107 (2)
N2—C10—C9	110.41 (18)	Sn—C14—H14	107 (3)
S1—C11—S2	117.04 (12)	Sn—C14—H14′	106 (3)
S1—C11—N3	119.91 (18)	C15—C14—H14	118 (3)
S2—C11—N3	123.05 (19)	C15—C14—H14′	109 (4)
Sn—C12—C13	118.10 (17)	H14—C14—H14′	102 (4)
Sn—C14—C15	114.2 (2)	C14—C15—H15	108 (4)
C1—C2—H2	119.1 (19)	C14—C15—H15′	113 (3)
C3—C2—H2	121.2 (19)	C14—C15—H15"	109 (3)
C2—C3—H3	118 (2)	H15—C15—H15′	107 (4)
C4—C3—H3	121 (2)	H15—C15—H15"	104 (4)
C4—C5—H5	123 (2)	H15′—C15—H15"	116 (4)

Cl—Sn—S1—C11	−177.91 (7)	C10—N2—C4—C3	−170.05 (18)
S2—Sn—S1—C11	0.63 (7)	C10—N2—C4—C5	13.5 (3)
C12—Sn—S1—C11	−86.14 (12)	C4—N2—C7—C8	−84.0 (2)
C14—Sn—S1—C11	84.39 (12)	C10—N2—C7—C8	60.9 (2)
Cl—Sn—S2—C11	3.03 (9)	C4—N2—C10—C9	81.7 (2)
S1—Sn—S2—C11	−0.64 (7)	C7—N2—C10—C9	−63.5 (2)
C12—Sn—S2—C11	117.96 (10)	C9—N3—C8—C7	51.0 (2)
C14—Sn—S2—C11	−117.45 (10)	C11—N3—C8—C7	−133.0 (2)
Cl—Sn—C12—C13	154.18 (19)	C8—N3—C9—C10	−52.7 (2)
S1—Sn—C12—C13	65.9 (2)	C11—N3—C9—C10	131.4 (2)
S2—Sn—C12—C13	−4.7 (2)	C8—N3—C11—S1	−169.60 (15)

C14—Sn—C12—C13	−103.9 (2)	C8—N3—C11—S2	10.3 (3)
Cl—Sn—C14—C15	148.7 (2)	C9—N3—C11—S1	6.0 (3)
S1—Sn—C14—C15	−120.6 (2)	C9—N3—C11—S2	−174.15 (16)
S2—Sn—C14—C15	−51.6 (2)	N1—C1—C2—C3	−178.72 (19)
C12—Sn—C14—C15	49.5 (3)	C6—C1—C2—C3	1.1 (3)
Sn—S1—C11—S2	−1.04 (11)	N1—C1—C6—C5	178.65 (19)
Sn—S1—C11—N3	178.87 (17)	C2—C1—C6—C5	−1.1 (3)
Sn—S2—C11—S1	0.96 (11)	C1—C2—C3—C4	0.0 (3)
Sn—S2—C11—N3	−178.95 (18)	C2—C3—C4—N2	−177.54 (19)
O1—N1—C1—C2	−178.47 (19)	C2—C3—C4—C5	−0.9 (3)
O1—N1—C1—C6	1.7 (3)	N2—C4—C5—C6	177.4 (2)
O2—N1—C1—C2	1.6 (3)	C3—C4—C5—C6	0.8 (3)
O2—N1—C1—C6	−178.2 (2)	C4—C5—C6—C1	0.2 (3)
C7—N2—C4—C3	−29.0 (3)	N2—C7—C8—N3	−54.2 (2)
C7—N2—C4—C5	154.5 (2)	N3—C9—C10—N2	58.6 (2)

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*, −*y*+3/2, *z*−1/2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) *x*, *y*+1, *z*; (viii) −*x*+1, *y*+1/2, −*z*+3/2; (ix) −*x*+1, −*y*+2, −*z*+1; (x) −*x*+1, *y*−1/2, −*z*+3/2; (xi) *x*, −*y*+3/2, *z*+1/2; (xii) *x*, *y*−1, *z*; (xiii) *x*, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1	0.87 (3)	2.43 (3)	2.737 (3)	101 (2)
C8—H8′···S2	0.95 (3)	2.52 (3)	3.067 (2)	117 (2)
C9—H9···S1	0.94 (3)	2.55 (2)	3.027 (2)	112.1 (19)