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The first example of a dinuclear organotin complex with a $C_2N_2S_2Sn_2$ planar dicyclo fragment

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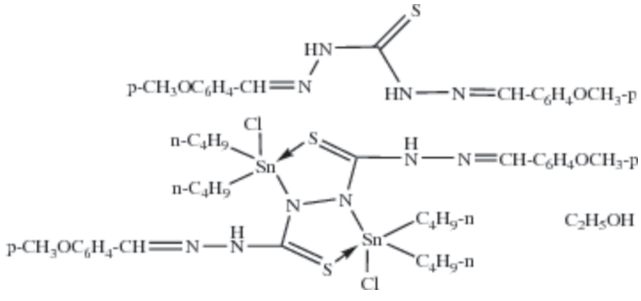
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.087; data-to-parameter ratio = 15.3.

The asymmetric unit of the unexpected title compound, 2,2,6,6-tetra-*n*-butyl-2,6-dichloro-4,8-bis{[(1*E*)-4-methoxybenzylidene]hydrazino}-1,5-diaza-2,6-distanna-3,7-dithiabicyclo[3.3.0]octa-3,7-diene bis{1,5[(1*E*)-4-methoxybenzylidene]thiocarbonohydrazide} ethanol disolvate, $[Sn_2(C_4H_9)_4Cl_2(C_{18}H_{18}N_6O_2S_2)]\cdot 2C_{17}H_{18}N_4O_2S\cdot 2C_2H_5OH$, comprises one half-molecule of the organotin complex, one thiocarbonohydrazide molecule and one ethanol solvent molecule, and is the first example of a substituted $C_2N_2S_2Sn_2$ planar dicyclo–organotin complex. Each Sn^{IV} atom is pentacoordinated with a distorted trigonal–bipyramidal geometry and the complex is disposed across a crystallographic centre of inversion. Weak intermolecular N—H···Cl and C—H···Cl hydrogen bonds and weak S···S interactions link the molecules of the organotin complex into one-dimensional infinite chains.

Related literature

For related literature, see: Altmann *et al.* (1998); Barbieri *et al.* (2001); Casas *et al.* (2000); Fang *et al.* (2001); Fang, Sui *et al.* (2006); Fang, Xu *et al.* (2006);Ma *et al.* (2005); Wang *et al.* (2004).



Experimental

Crystal data

$[Sn_2(C_4H_9)_4Cl_2(C_{18}H_{18}N_6O_2S_2)]\cdot\cdot 2C_{17}H_{18}N_4O_2S\cdot 2C_2H_6O$
M_r = 1728.20
Triclinic, $P\overline{1}$
a = 8.9295 (6) Å
b = 10.3932 (7) Å
c = 24.015 (2) Å
α = 81.439 (1)°
β = 85.350 (1)°
γ = 70.521 (1)°
V = 2076.6 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 296 (2) K
0.40 × 0.31 × 0.31 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.74, T_{max} = 0.77
13116 measured reflections
7145 independent reflections
6432 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.087
S = 1.04
7145 reflections
467 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C14	2.133 (3)	Sn1—S1	2.4717 (7)
Sn1—C10	2.140 (3)	Sn1—Cl1	2.6421 (7)
Sn1—N1	2.319 (2)	S1—C1	1.732 (2)
C14—Sn1—C10	147.6 (2)	N1—Sn1—S1	77.13 (6)
C14—Sn1—N1	96.5 (2)	C14—Sn1—Cl1	90.29 (9)
C10—Sn1—N1	95.9 (2)	C10—Sn1—Cl1	88.08 (8)
C14—Sn1—S1	105.58 (9)	N1—Sn1—Cl1	160.11 (6)
C10—Sn1—S1	106.3 (2)	S1—Sn1—Cl1	83.04 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N7	0.86	2.26	2.619 (4)	105
C2—H2A···Cl1^{i}	0.93	2.70	3.572 (3)	157
C25—H25···O4^{ii}	0.93	2.52	3.354 (5)	150
N2—H2···Cl1^{i}	0.86	2.62	3.398 (2)	151
N6—H6···S2^{iii}	0.86	2.53	3.386 (3)	171
N5—H5···O4^{ii}	0.86	2.62	3.379 (5)	147

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *APEX2*; program(s) used to refine structure: *APEX2*; molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2228).

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supplementary materials

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The first example of a dinuclear organotin complex with a $C_2N_2S_2Sn_2$ planar dicyclo fragment

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Comment

Organotin complexes have attracted attention in supermolecular chemistry in recent years (Ma *et al.*, 2005; Barbieri *et al.*, 2001), whereas thiosemicarbazones and their complexes have a wide range of applications in biology (Casas *et al.*, 2000). In the context of our continuous interest for the structural and biological properties of organotin compounds (Fang *et al.*, 2001; 2006a), we report here the crystal structure of the title complex, (I). To the best of our knowledge, this is the first example of organotin complex containing $C_2N_2S_2Sn_2$ planar dicyclo fragment.

The structure of (I) is an unexpected product in our work. It crystallizes in space group P-1, with one half-molecule of an organotin complex [2,2,6,6-Tetra-n-butyl-2,6-dichloro-4,8-di[(1E)-4-methoxybenzylidene]\ hydrazino-1,5-diaza-2,6-distanna-3,7-dithiabicyclo[3.3.0]octane], one substituted thiocarbonohydrazide ligand [1,5-Bis[(1E)-4-methoxybenzylidene]thiocarbonohydrazide] and one ethanol molecule in the asymmetric unit (Fig. 1). Part of the thiocarbonohydrazide ligand molecules were cracked to form a novel substituted $C_2N_2S_2Sn_2$ planar dicyclo organotin complex. The five-membered ring Sn1—S1—C1—N1A—N1 is coplanar with a mean deviation of 0.024 (3) Å. The inversion center is situated at the midpoint of N1—N1A bond, and it is by this bond that the two five-membered rings are fused together. Both of the Sn^{IV} atoms are penta-coordinated with distorted trigonal-bipyramidal geometry. C10, C14 (from butyl groups) and S1 atom occupy the equatorial plane, these equatorial atoms and relative Sn atom are nearly coplanar, the mean deviation from the plane is 0.031 (4) Å. Cl1 and N1 atoms occupy the axial positions with the N1—Sn1—Cl1 bond angle 160.11 (6)°. All the C═N bonds exist in E-configuration, and all the bond lengths in (I) are within the expected range and agree well with literature values (Altmann *et al.*, 1998; Fang *et al.*, 2006).

In the crystal lattice, every two molecules of the ligand are linked by the weak hydrogen bonds N6—H6···$S2^{i}$ to form dimers, with the attached two ethanol molecules by the strong N5—H5···$O4^{ii}$ and weak C25—H25···$O4^{ii}$ hydrogen bonds. The molecules of organotin are linked by S···S interactions (Wang *et al.*, 2004). and N—H···Cl^{iii}, C—H···Cl^{iii} weak hydrogen bonds involving all potential S and Cl atom donors, generating one-dimensional infinite chains parallel to the a axis, as shown in Fig. 2. The 4-methoxyphenyl rings protrude on both sides of these chains and have no special intercalations [symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x+1, -y+2, -z+1; (iii) -x+1, -y+2, -z].

Experimental

The title compound (I) was prepared as an unexpected product in our work by the following procedure: A solution of Schiff base ligand, 1,5-Bis[(1E)-4-methoxybenzylidene]thiocarbonohydrazide, (0.342 g, 1 m mol) and dibutyltin dichloride (0.304 g, 1 m mol) in acetonitrile (20 ml) was heated for 8 h under reflux. The reaction mixture was then cooled and the pale yellow precipitate that had formed was filtered off. Recrystallization of the crude product from ethanol-DMF solution resulted in single crystals of (I) suitable for X-ray diffraction analysis after several days.

Refinement

Slightly disorder in the ethanol was identified from the difference map. Disordered atoms were refined by applying restraints to the bond lengths [1.540 (2)Å for C35—C36 and 1.340 (2)Å for C35—O4]. All the H atoms were positioned in idealized locations and refined as riding on their carrier atoms, with O—H distances of 0.82 (hydroxyl), C—H distances of 0.93 (aryl), 0.97 (methylene) and 0.96Å (methyl) with Uiso(H) = 1.5Ueq(C) for hydroxyl and methyl, Uiso(H) = 1.2Ueq(C) for the other atoms.

Figures

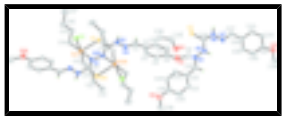


Fig.1. Molecular structure of (I), showing 25% probability displacement ellipsoids. H atoms not involved in hydrogen bonding have been omitted. The symmetry code for A is 2-x, 2-y, -z.

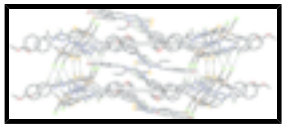


Fig.2. The packing of (I), viewed down the b axis, hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Table 1. Selected geometric parameters (Å, °).

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

2,2,6,6-Tetra-n-butyl-2,6-dichloro-4,8- bis{[(1E)-4-methoxybenzylidene]hydrazino}- 1,5-diaza-2,6-distanna-3,7-dithiabicyclo[3.3.0]octa-3,7-diene 1,5-bis[(1E)-4-methoxybenzylidene]thiocarbonohydrazide ethanol solvate

Crystal data

$[Sn_2(C_4H_9)_4Cl_2(C_{18}H_{18}N_6O_2S_2)]\cdot 2C_{17}H_{18}N_4O_2S\cdot 2C_2H_6O$	$Z = 1$
$M_r = 1728.20$	$F_{000} = 894$
Triclinic, $P\overline{1}$	$D_x = 1.382$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.9295$ (6) Å	Cell parameters from 9573 reflections
$b = 10.3932$ (7) Å	$\theta = 2.2$–$28.2°$
$c = 24.015$ (2) Å	$\mu = 0.83$ mm^{-1}
$\alpha = 81.439$ (1)°	$T = 296$ (2) K
$\beta = 85.350$ (1)°	Block, pale yellow
$\gamma = 70.521$ (1)°	0.40 × 0.31 × 0.31 mm
$V = 2076.6$ (3) Å^3	

Data collection

Bruker APEX II area-detector diffractometer	7145 independent reflections
Radiation source: fine-focus sealed tube	6432 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
$T = 296$(2) K	$\theta_{max} = 25.5°$
φ and ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -10\rightarrow 10$

T_{min} = 0.74, T_{max} = 0.77
13116 measured reflections

k = −12→12
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.087
S = 1.04
7145 reflections
467 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.6928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.812698 (18)	1.104088 (18)	−0.091670 (7)	0.04294 (8)
S1	0.70369 (8)	0.97683 (9)	−0.01266 (3)	0.05509 (19)
S2	0.60672 (15)	0.63859 (11)	0.44775 (4)	0.0835 (3)
O1	1.1578 (3)	0.6447 (3)	0.38324 (10)	0.0870 (8)
O2	1.0079 (4)	1.2706 (4)	0.32703 (14)	0.1100 (10)
O3	0.4216 (4)	0.6818 (3)	0.87416 (10)	0.0846 (7)
O4	0.4485 (5)	0.9813 (4)	0.38112 (15)	0.1195 (12)
H4A	0.5388	0.9519	0.3676	0.179*
N1	1.0120 (2)	1.0342 (2)	−0.02674 (9)	0.0428 (5)
N2	0.8235 (2)	0.8662 (3)	0.08325 (9)	0.0499 (5)
H2	0.7385	0.8437	0.0865	0.060*
N3	0.9227 (2)	0.8296 (2)	0.12835 (9)	0.0474 (5)
N4	0.6883 (3)	0.8739 (3)	0.47857 (11)	0.0608 (6)
N5	0.6294 (3)	0.7983 (3)	0.52189 (11)	0.0623 (6)

H5	0.6181	0.8206	0.5554	0.075*
N6	0.5359 (3)	0.6237 (3)	0.55591 (10)	0.0635 (7)
H6	0.5071	0.5548	0.5514	0.076*
N7	0.5255 (3)	0.6639 (3)	0.60890 (10)	0.0609 (6)
Cl1	0.53743 (9)	1.14405 (9)	−0.13637 (3)	0.0652 (2)
C1	0.8556 (3)	0.9364 (3)	0.03407 (10)	0.0408 (5)
C2	0.8603 (3)	0.7939 (3)	0.17573 (12)	0.0564 (7)
H2A	0.7561	0.7939	0.1760	0.068*
C3	0.9413 (3)	0.7534 (3)	0.22894 (12)	0.0556 (7)
C4	1.1033 (3)	0.7185 (3)	0.23344 (13)	0.0615 (8)
H4	1.1677	0.7184	0.2010	0.074*
C5	1.1705 (4)	0.6837 (4)	0.28516 (15)	0.0696 (9)
H5A	1.2801	0.6599	0.2874	0.084*
C6	1.0777 (4)	0.6836 (3)	0.33429 (14)	0.0654 (8)
C7	0.9148 (4)	0.7165 (4)	0.33124 (15)	0.0749 (10)
H7	0.8506	0.7157	0.3637	0.090*
C8	0.8499 (4)	0.7509 (4)	0.27789 (14)	0.0722 (9)
H8	0.7406	0.7730	0.2753	0.087*
C9	1.0686 (6)	0.6324 (5)	0.43472 (16)	0.1052 (15)
H9A	0.9938	0.7208	0.4404	0.158*
H9B	1.1396	0.5992	0.4655	0.158*
H9C	1.0126	0.5688	0.4329	0.158*
C10	0.7273 (4)	1.3153 (3)	−0.07763 (14)	0.0602 (7)
H10A	0.7475	1.3702	−0.1119	0.072*
H10B	0.6129	1.3418	−0.0715	0.072*
C11	0.7951 (4)	1.3536 (3)	−0.02949 (14)	0.0634 (8)
H11A	0.9084	1.3343	−0.0366	0.076*
H11B	0.7806	1.2959	0.0048	0.076*
C12	0.7209 (5)	1.5024 (4)	−0.02030 (19)	0.0827 (11)
H12A	0.7444	1.5594	−0.0534	0.099*
H12B	0.6064	1.5237	−0.0172	0.099*
C13	0.7737 (7)	1.5411 (6)	0.0304 (2)	0.1180 (18)
H13A	0.7333	1.4989	0.0638	0.177*
H13B	0.7340	1.6393	0.0295	0.177*
H13C	0.8877	1.5099	0.0304	0.177*
C14	0.9298 (4)	0.9572 (3)	−0.14765 (14)	0.0628 (8)
H14A	0.9071	1.0019	−0.1859	0.075*
H14B	1.0435	0.9324	−0.1435	0.075*
C15	0.8890 (5)	0.8280 (4)	−0.14076 (19)	0.0847 (11)
H15A	0.9100	0.7834	−0.1024	0.102*
H15B	0.7759	0.8519	−0.1460	0.102*
C16	0.9757 (6)	0.7283 (5)	−0.1798 (2)	0.0995 (14)
H16A	0.9539	0.7737	−0.2180	0.119*
H16B	1.0886	0.7064	−0.1748	0.119*
C17	0.9413 (8)	0.5976 (5)	−0.1746 (3)	0.130 (2)
H17A	0.9435	0.5587	−0.1357	0.194*
H17B	1.0200	0.5345	−0.1960	0.194*
H17C	0.8381	0.6146	−0.1888	0.194*
C18	1.0726 (9)	1.3605 (7)	0.3415 (3)	0.151 (3)

H18A	0.9978	1.4214	0.3648	0.226*
H18B	1.0990	1.4131	0.3081	0.226*
H18C	1.1672	1.3110	0.3620	0.226*
C19	0.9364 (5)	1.2028 (4)	0.37029 (17)	0.0806 (10)
C20	0.9198 (5)	1.2282 (4)	0.4242 (2)	0.0896 (12)
H20	0.9549	1.2957	0.4346	0.108*
C21	0.8485 (5)	1.1514 (4)	0.46519 (18)	0.0841 (11)
H21	0.8365	1.1685	0.5025	0.101*
C22	0.7980 (4)	1.0529 (3)	0.44951 (14)	0.0633 (8)
C23	0.8144 (4)	1.0330 (4)	0.39310 (15)	0.0739 (9)
H23	0.7773	0.9677	0.3817	0.089*
C24	0.8832 (5)	1.1063 (5)	0.35441 (18)	0.0852 (11)
H24	0.8939	1.0905	0.3170	0.102*
C25	0.7306 (4)	0.9690 (3)	0.49192 (14)	0.0636 (8)
H25	0.7188	0.9863	0.5292	0.076*
C26	0.5903 (4)	0.6915 (3)	0.51171 (13)	0.0595 (7)
C27	0.4748 (4)	0.5921 (3)	0.64858 (13)	0.0612 (7)
H27	0.4480	0.5182	0.6402	0.073*
C28	0.4574 (4)	0.6212 (3)	0.70636 (13)	0.0581 (7)
C29	0.4751 (5)	0.7397 (4)	0.72069 (14)	0.0690 (9)
H29	0.4951	0.8043	0.6925	0.083*
C30	0.4635 (5)	0.7629 (4)	0.77620 (14)	0.0720 (9)
H30	0.4748	0.8432	0.7852	0.086*
C31	0.4354 (4)	0.6676 (4)	0.81836 (13)	0.0630 (8)
C32	0.4171 (4)	0.5487 (4)	0.80527 (14)	0.0681 (9)
H32	0.3984	0.4840	0.8337	0.082*
C33	0.4268 (4)	0.5273 (4)	0.74950 (14)	0.0665 (8)
H33	0.4125	0.4482	0.7406	0.080*
C34	0.4351 (6)	0.8029 (4)	0.89018 (17)	0.0885 (12)
H34A	0.5373	0.8102	0.8778	0.133*
H34B	0.4242	0.7990	0.9304	0.133*
H34C	0.3531	0.8815	0.8732	0.133*
C35	0.3503 (8)	0.9364 (8)	0.3557 (2)	0.154 (3)
H35A	0.2418	0.9881	0.3658	0.185*
H35B	0.3677	0.8408	0.3706	0.185*
C36	0.3665 (12)	0.9471 (10)	0.2915 (2)	0.201 (4)
H36A	0.4087	1.0197	0.2772	0.302*
H36B	0.2640	0.9667	0.2762	0.302*
H36C	0.4370	0.8616	0.2807	0.302*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03414 (10)	0.04993 (13)	0.04704 (12)	−0.01539 (8)	−0.00385 (7)	−0.00810 (8)
S1	0.0380 (3)	0.0843 (5)	0.0499 (4)	−0.0309 (3)	−0.0072 (3)	−0.0015 (3)
S2	0.1316 (9)	0.0845 (7)	0.0550 (5)	−0.0642 (6)	0.0080 (5)	−0.0114 (4)
O1	0.0871 (18)	0.103 (2)	0.0635 (15)	−0.0213 (15)	−0.0233 (13)	−0.0003 (14)
O2	0.128 (3)	0.113 (3)	0.107 (2)	−0.072 (2)	0.0075 (19)	−0.0039 (19)

O3	0.117 (2)	0.0871 (18)	0.0569 (13)	−0.0421 (16)	0.0087 (13)	−0.0187 (12)
O4	0.123 (3)	0.144 (3)	0.108 (2)	−0.072 (3)	−0.032 (2)	0.016 (2)
N1	0.0316 (10)	0.0512 (13)	0.0465 (11)	−0.0142 (9)	−0.0047 (8)	−0.0061 (9)
N2	0.0348 (11)	0.0678 (15)	0.0511 (13)	−0.0232 (10)	−0.0059 (9)	−0.0025 (11)
N3	0.0385 (11)	0.0530 (13)	0.0531 (13)	−0.0184 (10)	−0.0079 (9)	−0.0023 (10)
N4	0.0718 (17)	0.0540 (15)	0.0574 (15)	−0.0246 (13)	0.0011 (12)	−0.0018 (12)
N5	0.0788 (18)	0.0582 (16)	0.0540 (14)	−0.0292 (14)	0.0021 (12)	−0.0066 (12)
N6	0.0831 (18)	0.0598 (16)	0.0535 (14)	−0.0322 (14)	0.0005 (12)	−0.0065 (12)
N7	0.0720 (17)	0.0575 (15)	0.0530 (14)	−0.0217 (13)	0.0003 (12)	−0.0060 (12)
Cl1	0.0440 (4)	0.0873 (6)	0.0691 (5)	−0.0273 (4)	−0.0169 (3)	−0.0028 (4)
C1	0.0319 (11)	0.0455 (14)	0.0467 (14)	−0.0142 (10)	−0.0009 (9)	−0.0072 (11)
C2	0.0452 (15)	0.069 (2)	0.0595 (17)	−0.0265 (14)	−0.0058 (12)	−0.0001 (14)
C3	0.0534 (16)	0.0594 (18)	0.0563 (17)	−0.0239 (14)	−0.0066 (12)	0.0010 (13)
C4	0.0484 (16)	0.072 (2)	0.0597 (18)	−0.0174 (15)	−0.0036 (13)	0.0017 (15)
C5	0.0524 (17)	0.080 (2)	0.072 (2)	−0.0189 (16)	−0.0111 (15)	0.0019 (17)
C6	0.070 (2)	0.061 (2)	0.0615 (19)	−0.0157 (16)	−0.0144 (15)	−0.0029 (15)
C7	0.067 (2)	0.088 (3)	0.060 (2)	−0.0150 (18)	−0.0011 (15)	−0.0042 (17)
C8	0.0495 (17)	0.094 (3)	0.068 (2)	−0.0219 (17)	−0.0037 (14)	0.0032 (18)
C9	0.124 (4)	0.117 (4)	0.054 (2)	−0.009 (3)	−0.013 (2)	−0.014 (2)
C10	0.0494 (16)	0.0533 (17)	0.075 (2)	−0.0076 (13)	−0.0078 (14)	−0.0172 (15)
C11	0.0637 (19)	0.0587 (19)	0.071 (2)	−0.0210 (15)	0.0015 (15)	−0.0193 (15)
C12	0.080 (2)	0.068 (2)	0.105 (3)	−0.0251 (19)	0.010 (2)	−0.032 (2)
C13	0.136 (4)	0.119 (4)	0.126 (4)	−0.061 (3)	0.028 (3)	−0.074 (3)
C14	0.0591 (18)	0.067 (2)	0.0679 (19)	−0.0245 (15)	0.0097 (14)	−0.0247 (16)
C15	0.091 (3)	0.074 (2)	0.099 (3)	−0.039 (2)	0.022 (2)	−0.031 (2)
C16	0.117 (4)	0.081 (3)	0.109 (3)	−0.036 (3)	0.020 (3)	−0.043 (3)
C17	0.165 (5)	0.089 (3)	0.153 (5)	−0.058 (4)	0.020 (4)	−0.050 (3)
C18	0.210 (7)	0.126 (5)	0.157 (5)	−0.114 (5)	−0.002 (5)	−0.002 (4)
C19	0.085 (3)	0.079 (3)	0.077 (2)	−0.031 (2)	−0.0040 (19)	0.006 (2)
C20	0.101 (3)	0.071 (2)	0.112 (3)	−0.049 (2)	−0.006 (2)	−0.012 (2)
C21	0.105 (3)	0.074 (2)	0.085 (3)	−0.046 (2)	−0.007 (2)	−0.007 (2)
C22	0.0634 (18)	0.0535 (18)	0.074 (2)	−0.0211 (15)	−0.0047 (15)	−0.0033 (15)
C23	0.080 (2)	0.075 (2)	0.071 (2)	−0.0339 (19)	0.0033 (17)	−0.0082 (18)
C24	0.091 (3)	0.094 (3)	0.077 (2)	−0.044 (2)	0.006 (2)	−0.006 (2)
C25	0.073 (2)	0.0599 (19)	0.0606 (18)	−0.0247 (16)	−0.0019 (15)	−0.0083 (15)
C26	0.0691 (19)	0.0536 (18)	0.0560 (17)	−0.0225 (15)	−0.0039 (14)	−0.0010 (14)
C27	0.072 (2)	0.0545 (18)	0.0591 (18)	−0.0241 (15)	0.0011 (14)	−0.0068 (14)
C28	0.0642 (18)	0.0535 (18)	0.0554 (17)	−0.0201 (14)	−0.0005 (13)	−0.0025 (13)
C29	0.093 (2)	0.059 (2)	0.0590 (19)	−0.0350 (18)	−0.0019 (16)	0.0014 (15)
C30	0.093 (3)	0.062 (2)	0.069 (2)	−0.0341 (19)	0.0013 (18)	−0.0119 (17)
C31	0.0655 (19)	0.066 (2)	0.0561 (18)	−0.0204 (16)	0.0046 (14)	−0.0095 (15)
C32	0.084 (2)	0.063 (2)	0.0586 (19)	−0.0298 (18)	0.0106 (16)	−0.0053 (15)
C33	0.077 (2)	0.059 (2)	0.067 (2)	−0.0284 (17)	0.0112 (16)	−0.0123 (16)
C34	0.109 (3)	0.088 (3)	0.074 (2)	−0.034 (2)	0.006 (2)	−0.029 (2)
C35	0.147 (6)	0.199 (8)	0.132 (5)	−0.087 (5)	−0.043 (4)	0.020 (5)
C36	0.276 (11)	0.247 (10)	0.162 (7)	−0.181 (9)	0.009 (7)	−0.060 (7)

Geometric parameters (Å, °)

Sn1—C14	2.133 (3)	C12—H12B	0.9700
Sn1—C10	2.140 (3)	C13—H13A	0.9600
Sn1—N1	2.319 (2)	C13—H13B	0.9600
Sn1—S1	2.4717 (7)	C13—H13C	0.9600
Sn1—Cl1	2.6421 (7)	C14—C15	1.488 (5)
S1—C1	1.732 (2)	C14—H14A	0.9700
S2—C26	1.687 (3)	C14—H14B	0.9700
O1—C6	1.364 (4)	C15—C16	1.479 (5)
O1—C9	1.428 (5)	C15—H15A	0.9700
O2—C18	1.349 (6)	C15—H15B	0.9700
O2—C19	1.399 (5)	C16—C17	1.475 (6)
O3—C31	1.361 (4)	C16—H16A	0.9700
O3—C34	1.413 (5)	C16—H16B	0.9700
O4—C35	1.343 (8)	C17—H17A	0.9600
O4—H4A	0.8200	C17—H17B	0.9600
N1—C1^{i}	1.309 (3)	C17—H17C	0.9600
N1—N1^{i}	1.409 (4)	C18—H18A	0.9600
N2—C1	1.355 (3)	C18—H18B	0.9600
N2—N3	1.382 (3)	C18—H18C	0.9600
N2—H2	0.8600	C19—C20	1.346 (6)
N3—C2	1.286 (4)	C19—C24	1.356 (6)
N4—C25	1.260 (4)	C20—C21	1.419 (6)
N4—N5	1.385 (4)	C20—H20	0.9300
N5—C26	1.329 (4)	C21—C22	1.358 (5)
N5—H5	0.8600	C21—H21	0.9300
N6—C26	1.335 (4)	C22—C23	1.389 (5)
N6—N7	1.384 (3)	C22—C25	1.465 (5)
N6—H6	0.8600	C23—C24	1.352 (5)
N7—C27	1.270 (4)	C23—H23	0.9300
C1—N1^{i}	1.309 (3)	C24—H24	0.9300
C2—C3	1.456 (4)	C25—H25	0.9300
C2—H2A	0.9300	C27—C28	1.449 (4)
C3—C8	1.378 (4)	C27—H27	0.9300
C3—C4	1.379 (4)	C28—C29	1.388 (5)
C4—C5	1.370 (4)	C28—C33	1.389 (5)
C4—H4	0.9300	C29—C30	1.379 (5)
C5—C6	1.386 (5)	C29—H29	0.9300
C5—H5A	0.9300	C30—C31	1.377 (5)
C6—C7	1.384 (5)	C30—H30	0.9300
C7—C8	1.397 (5)	C31—C32	1.382 (5)
C7—H7	0.9300	C32—C33	1.381 (5)
C8—H8	0.9300	C32—H32	0.9300
C9—H9A	0.9600	C33—H33	0.9300
C9—H9B	0.9600	C34—H34A	0.9600
C9—H9C	0.9600	C34—H34B	0.9600

C10—C11	1.507 (4)	C34—H34C	0.9600
C10—H10A	0.9700	C35—C36	1.528 (7)
C10—H10B	0.9700	C35—H35A	0.9700
C11—C12	1.509 (5)	C35—H35B	0.9700
C11—H11A	0.9700	C36—H36A	0.9600
C11—H11B	0.9700	C36—H36B	0.9600
C12—C13	1.493 (6)	C36—H36C	0.9600
C12—H12A	0.9700		
C14—Sn1—C10	147.6 (2)	H14A—C14—H14B	107.3
C14—Sn1—N1	96.5 (2)	C16—C15—C14	115.1 (3)
C10—Sn1—N1	95.9 (2)	C16—C15—H15A	108.5
C14—Sn1—S1	105.58 (9)	C14—C15—H15A	108.5
C10—Sn1—S1	106.3 (2)	C16—C15—H15B	108.5
N1—Sn1—S1	77.13 (6)	C14—C15—H15B	108.5
C14—Sn1—Cl1	90.29 (9)	H15A—C15—H15B	107.5
C10—Sn1—Cl1	88.08 (8)	C17—C16—C15	117.6 (4)
N1—Sn1—Cl1	160.11 (6)	C17—C16—H16A	107.9
S1—Sn1—Cl1	83.04 (2)	C15—C16—H16A	107.9
C1—S1—Sn1	99.19 (9)	C17—C16—H16B	107.9
C6—O1—C9	117.9 (3)	C15—C16—H16B	107.9
C18—O2—C19	117.2 (4)	H16A—C16—H16B	107.2
C31—O3—C34	118.2 (3)	C16—C17—H17A	109.5
C35—O4—H4A	109.5	C16—C17—H17B	109.5
$C1^{i}$—N1—$N1^{i}$	115.5 (2)	H17A—C17—H17B	109.5
$C1^{i}$—N1—Sn1	124.44 (18)	C16—C17—H17C	109.5
$N1^{i}$—N1—Sn1	119.78 (19)	H17A—C17—H17C	109.5
C1—N2—N3	122.2 (2)	H17B—C17—H17C	109.5
C1—N2—H2	118.9	O2—C18—H18A	109.5
N3—N2—H2	118.9	O2—C18—H18B	109.5
C2—N3—N2	115.0 (2)	H18A—C18—H18B	109.5
C25—N4—N5	116.5 (3)	O2—C18—H18C	109.5
C26—N5—N4	120.1 (3)	H18A—C18—H18C	109.5
C26—N5—H5	119.9	H18B—C18—H18C	109.5
N4—N5—H5	119.9	C20—C19—C24	120.7 (4)
C26—N6—N7	120.2 (3)	C20—C19—O2	124.2 (4)
C26—N6—H6	119.9	C24—C19—O2	115.1 (4)
N7—N6—H6	119.9	C19—C20—C21	119.8 (4)
C27—N7—N6	115.9 (3)	C19—C20—H20	120.1
$N1^{i}$—C1—N2	120.3 (2)	C21—C20—H20	120.1
$N1^{i}$—C1—S1	128.1 (2)	C22—C21—C20	119.5 (4)
N2—C1—S1	111.53 (17)	C22—C21—H21	120.3
N3—C2—C3	124.6 (3)	C20—C21—H21	120.3
N3—C2—H2A	117.7	C21—C22—C23	118.5 (3)
C3—C2—H2A	117.7	C21—C22—C25	119.9 (3)
C8—C3—C4	118.0 (3)	C23—C22—C25	121.6 (3)
C8—C3—C2	117.8 (3)	C24—C23—C22	121.5 (4)
C4—C3—C2	124.1 (3)	C24—C23—H23	119.2
C5—C4—C3	120.7 (3)	C22—C23—H23	119.2

C5—C4—H4	119.6	C23—C24—C19	120.0 (4)
C3—C4—H4	119.6	C23—C24—H24	120.0
C4—C5—C6	121.0 (3)	C19—C24—H24	120.0
C4—C5—H5A	119.5	N4—C25—C22	120.9 (3)
C6—C5—H5A	119.5	N4—C25—H25	119.6
O1—C6—C7	124.4 (3)	C22—C25—H25	119.6
O1—C6—C5	115.8 (3)	N5—C26—N6	116.2 (3)
C7—C6—C5	119.7 (3)	N5—C26—S2	124.2 (2)
C6—C7—C8	117.9 (3)	N6—C26—S2	119.6 (2)
C6—C7—H7	121.0	N7—C27—C28	122.4 (3)
C8—C7—H7	121.0	N7—C27—H27	118.8
C3—C8—C7	122.6 (3)	C28—C27—H27	118.8
C3—C8—H8	118.7	C29—C28—C33	118.0 (3)
C7—C8—H8	118.7	C29—C28—C27	121.8 (3)
O1—C9—H9A	109.5	C33—C28—C27	120.1 (3)
O1—C9—H9B	109.5	C30—C29—C28	120.8 (3)
H9A—C9—H9B	109.5	C30—C29—H29	119.6
O1—C9—H9C	109.5	C28—C29—H29	119.6
H9A—C9—H9C	109.5	C31—C30—C29	120.2 (3)
H9B—C9—H9C	109.5	C31—C30—H30	119.9
C11—C10—Sn1	117.4 (2)	C29—C30—H30	119.9
C11—C10—H10A	107.9	O3—C31—C30	124.3 (3)
Sn1—C10—H10A	107.9	O3—C31—C32	115.5 (3)
C11—C10—H10B	107.9	C30—C31—C32	120.2 (3)
Sn1—C10—H10B	107.9	C33—C32—C31	119.2 (3)
H10A—C10—H10B	107.2	C33—C32—H32	120.4
C10—C11—C12	113.9 (3)	C31—C32—H32	120.4
C10—C11—H11A	108.8	C32—C33—C28	121.6 (3)
C12—C11—H11A	108.8	C32—C33—H33	119.2
C10—C11—H11B	108.8	C28—C33—H33	119.2
C12—C11—H11B	108.8	O3—C34—H34A	109.5
H11A—C11—H11B	107.7	O3—C34—H34B	109.5
C13—C12—C11	115.5 (4)	H34A—C34—H34B	109.5
C13—C12—H12A	108.4	O3—C34—H34C	109.5
C11—C12—H12A	108.4	H34A—C34—H34C	109.5
C13—C12—H12B	108.4	H34B—C34—H34C	109.5
C11—C12—H12B	108.4	O4—C35—C36	116.3 (5)
H12A—C12—H12B	107.5	O4—C35—H35A	108.2
C12—C13—H13A	109.5	C36—C35—H35A	108.2
C12—C13—H13B	109.5	O4—C35—H35B	108.2
H13A—C13—H13B	109.5	C36—C35—H35B	108.2
C12—C13—H13C	109.5	H35A—C35—H35B	107.4
H13A—C13—H13C	109.5	C35—C36—H36A	109.5
H13B—C13—H13C	109.5	C35—C36—H36B	109.5
C15—C14—Sn1	117.1 (2)	H36A—C36—H36B	109.5
C15—C14—H14A	108.0	C35—C36—H36C	109.5
Sn1—C14—H14A	108.0	H36A—C36—H36C	109.5
C15—C14—H14B	108.0	H36B—C36—H36C	109.5
Sn1—C14—H14B	108.0		

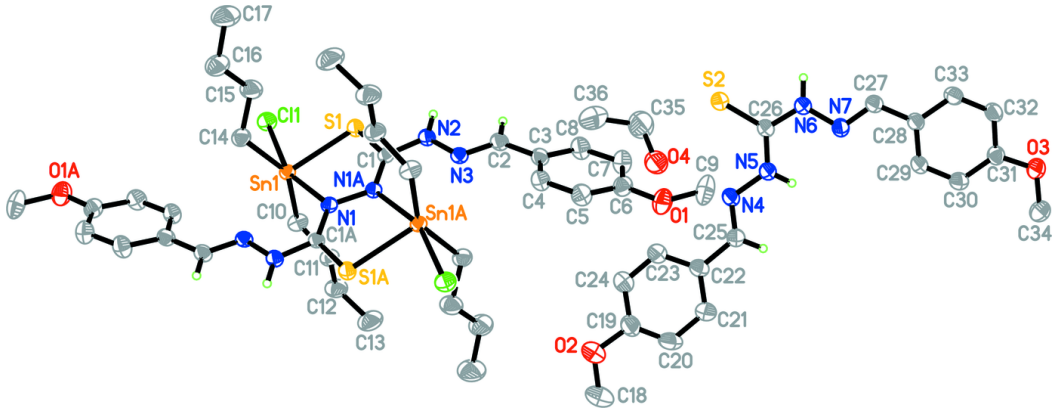
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N7	0.86	2.26	2.619 (4)	105
C2—H2A···Cl1^{ii}	0.93	2.70	3.572 (3)	157
C25—H25···O4^{iii}	0.93	2.52	3.354 (5)	150
N2—H2···Cl1^{ii}	0.86	2.62	3.398 (2)	151
N6—H6···S2^{iv}	0.86	2.53	3.386 (3)	171
N5—H5···O4^{iii}	0.86	2.62	3.379 (5)	147

Symmetry codes: (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C17
C16
C15
C14
Cl1
S1
N2
C1
N3
C2
C3
C8
C36
C35
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C7
C9
N5
S2
C26
N6
N7
C27
C33
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C28
C29
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O3
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C5
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N4
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C10
N1
C1A
Sn1A
C11
S1A
C12
C13
C24
C23
C22
C21
C19
C20
O2
C18

Fig. 2