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Dichloridobis(dimethyl sulfoxide-κO)-diphenyltin(IV)

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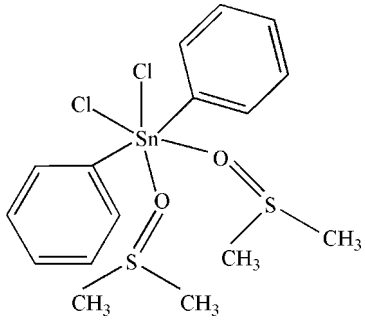
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.021; wR factor = 0.048; data-to-parameter ratio = 13.8.

The geometry around the Sn atom of the title compound, $[Sn(C_6H_5)_2Cl_2(C_2H_6OS)_2]$, is distorted octahedral, with Sn—C and Sn—O distances lying in the ranges 2.139 (4)–2.156 (4) and 2.270 (2)–2.279 (2) Å, respectively. Molecules are linked by intermolecular C—H···O and C—H···Cl hydrogen bonds, and by C—H···π interactions with distances of 2.8 and 2.75 Å.

Related literature

For related literature, see: Anderson *et al.* (1984); Gielen (1994); McManus *et al.* (1994); Nath *et al.* (2001); Ng *et al.* (1991); Selvaratnam *et al.* (1994); Shahzadi *et al.* (2006); Xie *et al.* (1996).



Experimental

Crystal data

$[Sn(C_6H_5)_2Cl_2(C_2H_6OS)_2]$
M_r = 500.05
Monoclinic, Pn
a = 9.8877 (8) Å
b = 7.9766 (6) Å
c = 12.5880 (10) Å
β = 95.5060 (10)°
V = 988.24 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.78 mm^{-1}
T = 100 (2) K
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.536, T_{max} = 0.717
5514 measured reflections
2934 independent reflections
2884 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.048
S = 1.05
2934 reflections
212 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Absolute structure: Flack (1983), 917 Freidel pairs
Flack parameter: 0.024 (17)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···O1^{i}	0.98	2.39	3.260 (5)	148
C3—H3···Cl2^{ii}	0.95	2.79	3.721 (4)	166
C14—H14B···Cl2^{iii}	0.98	2.73	3.663 (4)	160

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2303).

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supplementary materials

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Dichloridobis(dimethyl sulfoxide-*κO*)diphenyltin(IV)

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Comment

There have been several reports dealing with the impact of organotin chemistry in the biosphere (Gielen, 1994; Ng *et al.*, 1991). Exploration of the structural-activity relationships of such systems has led to numerous reports in recent years (Gielen, 1994; Selvaratnam *et al.*, 1994; McManus *et al.*, 1994). Organotin compounds are of current interest due to their dramatic increase of industrial, agricultural and biological applications (Xie *et al.*, 1996; Nath *et al.*, 2001). The studies of organotin and biologically important ligands have gained importance due to potential pharmaceutical applications of organotin compounds (Anderson *et al.*, 1984). We report here the crystal structure of the title compound (I) as a continuation of our efforts in the synthesis and structural characterization of organotin(IV) complexes (Shahzadi *et al.*, 2006) (Fig 1).

The Sn atom is bonded to two phenyls, two DMSO groups and two chlorides forming a distorted octahedral geometry. The Sn—C distances lie in the range 2.139 (4) − 2.156 (4) Å which is longer than Sn—C distance reported earlier (Shahzadi *et al.*, 2006). The C1—Sn1—C7 and O1—Sn1—Cl2 angles are 172.19 (3) and 170.97 (6)°, respectively (Table 1). The molecules are linked by C—H···O and C—H···Cl hydrogen bonds (Table 1, Fig.2) and C—H···π interactions between H11—*Cg*1 (symmetry equivalent −1 + *x*, *y*, *z*) and H13A and *Cg*2 (symmetry equivalent 1/2 + *x*, 1 − *y*, −1/2 + *z*) with distances of 2.8 and 2.75, where *Cg*1 and *Cg*2 are the phenyl rings C1—C6 and C7—C12, respectively.

Experimental

1-(2-Pyridyl)piperazine (2 mmol), carbondisulfide (2 mmol) and diphenyltin dichloride (1 mmol) were suspended in dry methanol (150 ml) in a two necked round bottom flask. The mixture was stirred at room temperature for 24 h. Solid product obtained was filtered off and recrystallized from DMSO to obtain colourless crystals suitable for X-ray analysis (yield 65%; m.p. 414–416 K).

Refinement

H atoms were included in calculated positions using the riding method, with C—H = 0.95 − 0.98 Å and U_{eq} values 1.2 times those of the parent atoms (1.5 times those of the methyl C atoms).

Figures

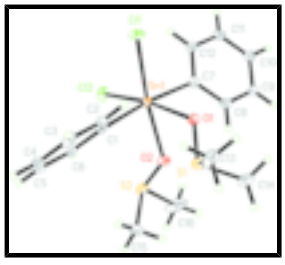

Fig. 1. Structure of (I) with displacement ellipsoids drawn at the 50% probability level.

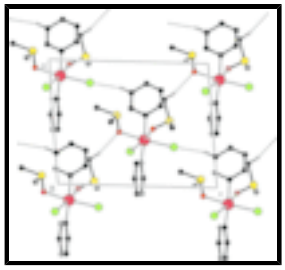

Fig. 2. Packing of (I) viewed down the *b* axis showing the hydrogen bonding interactions with dotted lines..

Dichloridobis(dimethyl sulfoxide-κ*O*)diphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_2Cl_2(C_2H_6OS)_2]$	F_{000} = 500
M_r = 500.05	D_x = 1.680 Mg m^{-3}
Monoclinic, *Pn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yac	Cell parameters from 3405 reflections
a = 9.8877 (8) Å	θ = 2.5–26.4º
b = 7.9766 (6) Å	μ = 1.78 mm^{-1}
c = 12.5880 (10) Å	*T* = 100 (2) K
β = 95.5060 (10)º	Rectangular, colourless
V = 988.24 (13) Å^3	0.40 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	2934 independent reflections
Radiation source: fine-focus sealed tube	2884 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 100(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −12→8
T_{min} = 0.536, T_{max} = 0.717	*k* = −9→9
5514 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.021	$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.048	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.63 e Å^{-3}
2934 reflections	$\Delta\rho_{min}$ = −0.50 e Å^{-3}

212 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: none

Absolute structure: Flack (1983), with 917 Freidel pairs

Flack parameter: 0.024 (17)

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 $F^2 > \sigma(F^2)$ 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	0.87116 (2)	0.73205 (2)	0.06392 (2)	0.01157 (6)
S1	1.06401 (9)	0.52499 (11)	−0.09835 (7)	0.01579 (19)
S2	1.02952 (11)	0.42840 (11)	0.23125 (7)	0.0206 (2)
Cl1	0.77624 (10)	0.98627 (11)	−0.02938 (7)	0.01949 (19)
Cl2	0.82060 (10)	0.81165 (12)	0.24691 (7)	0.0198 (2)
O1	0.9310 (2)	0.6217 (3)	−0.09105 (19)	0.0155 (5)
O2	0.9624 (3)	0.4828 (3)	0.1231 (2)	0.0210 (6)
C1	1.0711 (4)	0.8424 (4)	0.0825 (3)	0.0127 (7)
C2	1.1228 (4)	0.9177 (4)	−0.0049 (3)	0.0159 (8)
H2	1.0705	0.9166	−0.0722	0.019*
C3	1.2497 (4)	0.9946 (4)	0.0047 (3)	0.0189 (8)
H3	1.2844	1.0428	−0.0562	0.023*
C4	1.3253 (4)	1.0006 (4)	0.1028 (3)	0.0189 (8)
H4	1.4115	1.0541	0.1096	0.023*
C5	1.2750 (4)	0.9282 (4)	0.1915 (3)	0.0167 (8)
H5	1.3270	0.9327	0.2590	0.020*
C6	1.1492 (4)	0.8494 (4)	0.1819 (3)	0.0149 (7)
H6	1.1156	0.8000	0.2428	0.018*
C7	0.6846 (4)	0.5975 (4)	0.0322 (3)	0.0147 (7)
C8	0.6804 (4)	0.4271 (4)	0.0050 (3)	0.0154 (7)
H8	0.7629	0.3683	−0.0009	0.019*
C9	0.5576 (4)	0.3430 (5)	−0.0136 (3)	0.0175 (8)
H9	0.5566	0.2275	−0.0321	0.021*
C10	0.4357 (4)	0.4273 (4)	−0.0052 (3)	0.0166 (8)
H10	0.3515	0.3700	−0.0180	0.020*
C11	0.4387 (4)	0.5969 (5)	0.0224 (3)	0.0190 (8)
H11	0.3563	0.6555	0.0291	0.023*

C12	0.5621 (4)	0.6799 (5)	0.0400 (3)	0.0168 (8)
H12	0.5629	0.7957	0.0578	0.020*
C13	1.1218 (4)	0.5947 (5)	−0.2208 (3)	0.0245 (9)
H13A	1.0480	0.5843	−0.2782	0.037*
H13B	1.1990	0.5258	−0.2377	0.037*
H13C	1.1502	0.7122	−0.2139	0.037*
C14	1.0108 (4)	0.3205 (5)	−0.1386 (3)	0.0228 (8)
H14A	0.9738	0.2631	−0.0789	0.034*
H14B	1.0886	0.2573	−0.1603	0.034*
H14C	0.9405	0.3281	−0.1989	0.034*
C15	1.2005 (5)	0.3876 (6)	0.2057 (4)	0.0369 (11)
H15A	1.2014	0.3062	0.1474	0.055*
H15B	1.2508	0.3421	0.2701	0.055*
H15C	1.2433	0.4921	0.1854	0.055*
C16	0.9765 (6)	0.2180 (5)	0.2451 (5)	0.0407 (13)
H16A	0.8812	0.2161	0.2604	0.061*
H16B	1.0329	0.1647	0.3039	0.061*
H16C	0.9861	0.1569	0.1787	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01164 (11)	0.01114 (10)	0.01229 (10)	0.00108 (13)	0.00299 (7)	−0.00024 (13)
S1	0.0119 (4)	0.0192 (4)	0.0167 (4)	0.0013 (4)	0.0036 (3)	−0.0044 (3)
S2	0.0318 (6)	0.0153 (5)	0.0153 (4)	0.0075 (4)	0.0047 (4)	0.0014 (3)
Cl1	0.0171 (5)	0.0160 (4)	0.0259 (4)	0.0041 (3)	0.0045 (4)	0.0067 (3)
Cl2	0.0225 (5)	0.0229 (5)	0.0153 (4)	−0.0040 (4)	0.0088 (4)	−0.0041 (3)
O1	0.0127 (13)	0.0181 (13)	0.0159 (12)	0.0018 (10)	0.0027 (10)	−0.0040 (10)
O2	0.0231 (16)	0.0156 (13)	0.0231 (14)	0.0049 (12)	−0.0045 (11)	0.0003 (10)
C1	0.0123 (18)	0.0096 (16)	0.0163 (17)	0.0028 (14)	0.0022 (14)	−0.0031 (13)
C2	0.018 (2)	0.0145 (18)	0.0164 (18)	0.0027 (15)	0.0050 (15)	−0.0024 (14)
C3	0.026 (2)	0.0113 (17)	0.0206 (18)	−0.0011 (15)	0.0098 (15)	0.0023 (14)
C4	0.015 (2)	0.0116 (17)	0.030 (2)	−0.0018 (15)	0.0049 (16)	−0.0027 (15)
C5	0.016 (2)	0.0133 (17)	0.0198 (18)	0.0054 (15)	−0.0026 (15)	−0.0022 (14)
C6	0.0189 (19)	0.0115 (17)	0.0147 (17)	0.0029 (14)	0.0042 (14)	−0.0022 (13)
C7	0.0170 (19)	0.0164 (18)	0.0113 (16)	0.0010 (15)	0.0050 (14)	0.0024 (13)
C8	0.0149 (19)	0.0170 (18)	0.0147 (17)	0.0025 (15)	0.0034 (14)	0.0019 (14)
C9	0.020 (2)	0.0125 (18)	0.0206 (18)	0.0025 (15)	0.0033 (16)	0.0005 (15)
C10	0.0115 (19)	0.0183 (18)	0.0205 (18)	−0.0047 (14)	0.0041 (15)	−0.0003 (14)
C11	0.0122 (19)	0.0211 (19)	0.0242 (19)	0.0041 (15)	0.0036 (15)	0.0018 (15)
C12	0.016 (2)	0.0148 (18)	0.0201 (18)	0.0009 (15)	0.0039 (15)	−0.0001 (14)
C13	0.027 (2)	0.024 (2)	0.025 (2)	−0.0026 (17)	0.0149 (18)	−0.0065 (16)
C14	0.021 (2)	0.0165 (19)	0.032 (2)	0.0020 (16)	0.0081 (17)	0.0010 (16)
C15	0.020 (2)	0.025 (2)	0.061 (3)	0.0036 (19)	−0.015 (2)	0.002 (2)
C16	0.038 (3)	0.020 (2)	0.069 (4)	0.007 (2)	0.031 (3)	0.018 (2)

Geometric parameters (Å, °)

Sn1—C7	2.139 (4)	C7—C12	1.390 (5)

Sn1—C1	2.156 (4)	C7—C8	1.402 (5)
Sn1—O1	2.270 (2)	C8—C9	1.387 (5)
Sn1—O2	2.279 (2)	C8—H8	0.9500
Sn1—Cl1	2.4821 (9)	C9—C10	1.393 (5)
Sn1—Cl2	2.4860 (9)	C9—H9	0.9500
S1—O1	1.535 (3)	C10—C11	1.397 (5)
S1—C14	1.773 (4)	C10—H10	0.9500
S1—C13	1.784 (4)	C11—C12	1.387 (5)
S2—O2	1.519 (3)	C11—H11	0.9500
S2—C16	1.772 (4)	C12—H12	0.9500
S2—C15	1.781 (5)	C13—H13A	0.9800
C1—C2	1.393 (5)	C13—H13B	0.9800
C1—C6	1.407 (5)	C13—H13C	0.9800
C2—C3	1.391 (5)	C14—H14A	0.9800
C2—H2	0.9500	C14—H14B	0.9800
C3—C4	1.381 (6)	C14—H14C	0.9800
C3—H3	0.9500	C15—H15A	0.9800
C4—C5	1.391 (5)	C15—H15B	0.9800
C4—H4	0.9500	C15—H15C	0.9800
C5—C6	1.389 (5)	C16—H16A	0.9800
C5—H5	0.9500	C16—H16B	0.9800
C6—H6	0.9500	C16—H16C	0.9800
C7—Sn1—C1	172.19 (13)	C12—C7—Sn1	119.4 (3)
C7—Sn1—O1	86.36 (11)	C8—C7—Sn1	122.5 (3)
C1—Sn1—O1	86.54 (11)	C9—C8—C7	121.0 (4)
C7—Sn1—O2	86.02 (12)	C9—C8—H8	119.5
C1—Sn1—O2	89.46 (11)	C7—C8—H8	119.5
O1—Sn1—O2	79.35 (9)	C8—C9—C10	120.2 (3)
C7—Sn1—Cl1	92.38 (10)	C8—C9—H9	119.9
C1—Sn1—Cl1	91.08 (9)	C10—C9—H9	119.9
O1—Sn1—Cl1	91.61 (6)	C9—C10—C11	119.2 (4)
O2—Sn1—Cl1	170.89 (7)	C9—C10—H10	120.4
C7—Sn1—Cl2	93.11 (10)	C11—C10—H10	120.4
C1—Sn1—Cl2	93.38 (9)	C12—C11—C10	120.0 (4)
O1—Sn1—Cl2	170.97 (6)	C12—C11—H11	120.0
O2—Sn1—Cl2	91.62 (7)	C10—C11—H11	120.0
Cl1—Sn1—Cl2	97.42 (3)	C11—C12—C7	121.5 (3)
O1—S1—C14	104.30 (17)	C11—C12—H12	119.3
O1—S1—C13	104.04 (16)	C7—C12—H12	119.3
C14—S1—C13	98.65 (19)	S1—C13—H13A	109.5
O2—S2—C16	104.5 (2)	S1—C13—H13B	109.5
O2—S2—C15	103.3 (2)	H13A—C13—H13B	109.5
C16—S2—C15	98.0 (2)	S1—C13—H13C	109.5
S1—O1—Sn1	122.81 (13)	H13A—C13—H13C	109.5
S2—O2—Sn1	131.88 (15)	H13B—C13—H13C	109.5
C2—C1—C6	118.2 (3)	S1—C14—H14A	109.5
C2—C1—Sn1	119.5 (3)	S1—C14—H14B	109.5
C6—C1—Sn1	122.1 (3)	H14A—C14—H14B	109.5
C3—C2—C1	121.2 (3)	S1—C14—H14C	109.5

C3—C2—H2	119.4	H14A—C14—H14C	109.5
C1—C2—H2	119.4	H14B—C14—H14C	109.5
C4—C3—C2	119.9 (3)	S2—C15—H15A	109.5
C4—C3—H3	120.0	S2—C15—H15B	109.5
C2—C3—H3	120.0	H15A—C15—H15B	109.5
C3—C4—C5	120.0 (4)	S2—C15—H15C	109.5
C3—C4—H4	120.0	H15A—C15—H15C	109.5
C5—C4—H4	120.0	H15B—C15—H15C	109.5
C6—C5—C4	120.2 (3)	S2—C16—H16A	109.5
C6—C5—H5	119.9	S2—C16—H16B	109.5
C4—C5—H5	119.9	H16A—C16—H16B	109.5
C5—C6—C1	120.4 (3)	S2—C16—H16C	109.5
C5—C6—H6	119.8	H16A—C16—H16C	109.5
C1—C6—H6	119.8	H16B—C16—H16C	109.5
C12—C7—C8	118.1 (4)		
C14—S1—O1—Sn1	117.33 (19)	C1—C2—C3—C4	−1.6 (5)
C13—S1—O1—Sn1	−139.74 (17)	C2—C3—C4—C5	0.7 (5)
C7—Sn1—O1—S1	−126.56 (18)	C3—C4—C5—C6	0.2 (5)
C1—Sn1—O1—S1	50.17 (17)	C4—C5—C6—C1	−0.2 (5)
O2—Sn1—O1—S1	−39.93 (16)	C2—C1—C6—C5	−0.6 (5)
Cl1—Sn1—O1—S1	141.16 (15)	Sn1—C1—C6—C5	−177.1 (3)
C16—S2—O2—Sn1	143.5 (2)	O1—Sn1—C7—C12	−131.5 (3)
C15—S2—O2—Sn1	−114.4 (2)	O2—Sn1—C7—C12	148.9 (3)
C7—Sn1—O2—S2	−119.4 (2)	Cl1—Sn1—C7—C12	−40.0 (3)
C1—Sn1—O2—S2	67.0 (2)	Cl2—Sn1—C7—C12	57.5 (3)
O1—Sn1—O2—S2	153.6 (2)	O1—Sn1—C7—C8	49.3 (3)
Cl2—Sn1—O2—S2	−26.4 (2)	O2—Sn1—C7—C8	−30.2 (3)
O1—Sn1—C1—C2	43.7 (3)	Cl1—Sn1—C7—C8	140.8 (3)
O2—Sn1—C1—C2	123.1 (3)	Cl2—Sn1—C7—C8	−121.6 (3)
Cl1—Sn1—C1—C2	−47.8 (3)	C12—C7—C8—C9	−0.1 (5)
Cl2—Sn1—C1—C2	−145.3 (3)	Sn1—C7—C8—C9	179.1 (3)
O1—Sn1—C1—C6	−139.8 (3)	C7—C8—C9—C10	−0.1 (5)
O2—Sn1—C1—C6	−60.5 (3)	C8—C9—C10—C11	−0.2 (5)
Cl1—Sn1—C1—C6	128.6 (3)	C9—C10—C11—C12	0.6 (6)
Cl2—Sn1—C1—C6	31.1 (3)	C10—C11—C12—C7	−0.8 (6)
C6—C1—C2—C3	1.5 (5)	C8—C7—C12—C11	0.6 (5)
Sn1—C1—C2—C3	178.1 (3)	Sn1—C7—C12—C11	−178.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···O1^{i}	0.98	2.39	3.260 (5)	148
C3—H3···Cl2^{ii}	0.95	2.79	3.721 (4)	166
C14—H14B···Cl2^{iii}	0.98	2.73	3.663 (4)	160

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

Fig. 1

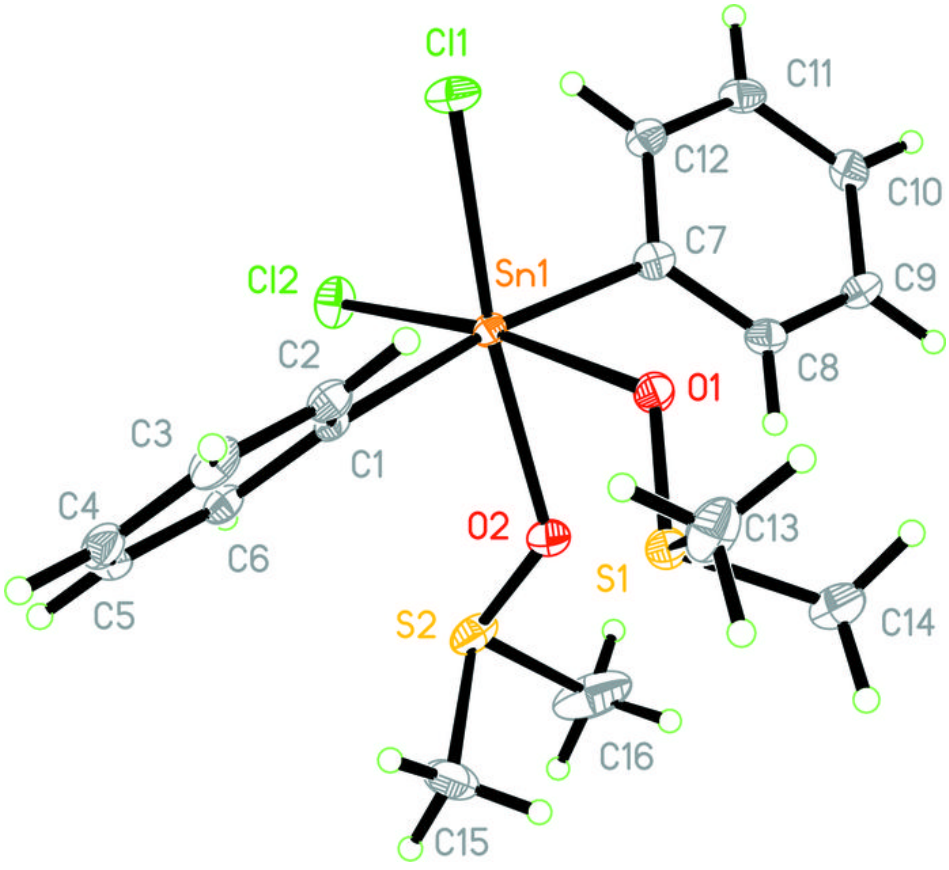
Cl1
C11
C12
C10
C7
Cl2
Sn1
C9
C2
C8
O1
C3
C1
C4
O2
C13
C6
S1
S2
C14
C5
C16
C15

Fig. 2