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Octakis(2-chlorobenzyl)di-μ_2-hydroxido-di-μ_3-oxido-bis(2-phenylacetato)tetra-tin(IV)

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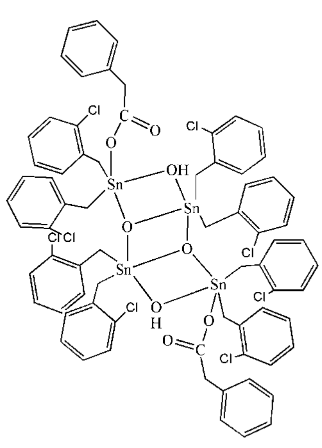
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.040; wR factor = 0.121; data-to-parameter ratio = 15.2.

The asymmetric unit of the title compound, $[Sn_4(C_7H_6Cl)_8(C_8H_7O_2)_2O_2(OH)_2]$, comprises one-half of the centrosymmetric tin(IV) complex. μ_3-Oxide and μ_2-hydroxide bridges link the four five-coordinate Sn^{IV} atoms to generate three fused four-membered Sn—O—Sn—O rings in a ladder-like structure. The two endocyclic Sn atoms each bind to two μ_3-oxide anions and a μ_2-hydroxide ligand, together with two 2-chlorobenzyl groups. The exocyclic Sn atoms each carry a monodentate phenylacetate ligand, two 2-chlorobenzyl groups, and μ_3-oxide and μ_2-hydroxide ligands. Both types of Sn atoms adopt a distorted trigonal–bipyramidal coordination geometry. The molecular conformation is stabilized by intramolecular O—H···O interactions involving the μ_2-hydroxide ligands and the C═O group of the phenylacetate ligand.

Related literature

For the antifungal activity of organotin compounds, see: Ruzicka *et al.* (2002); Nath *et al.* (1999). For a related structure, see: Wu *et al.* (2009).



Experimental

Crystal data

$[Sn_4(C_7H_6Cl)_8(C_8H_7O_2)_2O_2(OH)_2]$
M_r = 1815.59
Triclinic, $P\overline{1}$
a = 10.7095 (14) Å
b = 11.4846 (16) Å
c = 15.2412 (18) Å
α = 98.311 (2)°
β = 90.982 (1)°
γ = 98.404 (2)°
V = 1833.6 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 298 K
0.49 × 0.48 × 0.40 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) T_{min} = 0.491, T_{max} = 0.551
9422 measured reflections
6322 independent reflections
4437 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.121
S = 1.05
6322 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O3	2.023 (4)	Sn2—O4	2.033 (4)
Sn1—O2	2.114 (4)	Sn2—O4^i	2.089 (3)
Sn1—C9	2.145 (6)	Sn2—C30	2.146 (6)
Sn1—C16	2.145 (7)	Sn2—O3	2.163 (4)
Sn1—O4	2.157 (3)	Sn2—C23	2.165 (6)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1	0.82	1.78	2.554 (7)	157

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2764).

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supplementary materials

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Octakis(2-chlorobenzyl)di-μ_2-hydroxido-di-μ_3-oxido-bis(2-phenylacetato)tetratin(IV)

W.-B. Peng, G.-Q. Li, H. Yin and X. Zhao

Comment

Recently considerable attention has been paid to organotin(IV) derivatives, owing to their high in vitro antifungal activities against some medically important fungi (Ruzicka *et al.*, 2002; Nath *et al.*, 1999). As a continuation of our study of organotin compounds, we present here the synthesis and crystal structure of the title compound (I).

The title compound (Fig. 1, Table 1) is a centrosymmetric dimer and displays a ladder type structural motif. The ladder consists of four tin centers held together by two μ_3-oxygen atoms. According to their different coordination environments, the four tin atoms can be divided into two types, viz. two endocyclic and two exocyclic. The endo- and exocyclic tin centers are linked by μ_2-hydroxide anions and μ_3-oxide anions. Each of the tin atoms is five-coordinate, adopting approximate trigonal bipyramidal coordination. The 2-phenylacetato ligands coordinate to the exocyclic tin atoms in a monodentate fashion, and the molecular conformation is stabilized by intramolecular O3—H3···O1 hydrogen bonds (Table 2). The crystal structure of a similiar compound has been reported recently (Wu *et al.*, 2009).

Experimental

The reaction was carried out under a nitrogen atmosphere. 2-phenylacetic acid (2 mmol) and sodium ethoxide (2.2 mmol) were added to a stirred solution of benzene (30 ml) in a Schlenk flask and stirred for 0.5 h. Bis(2-chlorobenzyl)dichlorostannane (4 mmol) was then added to the reactor. After stirring for 10 h at 323 K, a white paste was obtained and filtered off. Colourless crystals suitable for X-ray analysis were obtained by slow evaporation of dichloromethane/methanol (1:1 v/v) solution over a period of six days (yield 86%. m.p. 438 K).

Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and O—H = 0.82 Å for aromatic, methylene and hydroxyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O) for hydroxyl groups

Figures

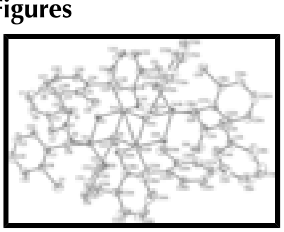


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

Octakis(2-chlorobenzyl)di-μ$_2$-hydroxido-di-μ$_3$-oxido- bis(2-phenylacetato)tetratin(IV)

Crystal data

$[Sn_4(C_7H_6Cl)_8(C_8H_7O_2)_2O_2(OH)_2]$	$Z = 1$
$M_r = 1815.59$	$F(000) = 896$
Triclinic, $P\overline{1}$	$D_x = 1.644$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.7095$ (14) Å	Cell parameters from 4098 reflections
$b = 11.4846$ (16) Å	$\theta = 2.3$–27.0°
$c = 15.2412$ (18) Å	$\mu = 1.69$ mm^{-1}
$\alpha = 98.311$ (2)°	$T = 298$ K
$\beta = 90.982$ (1)°	Block, colourless
$\gamma = 98.404$ (2)°	0.49 × 0.48 × 0.40 mm
$V = 1833.6$ (4) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	6322 independent reflections
Radiation source: fine-focus sealed tube	4437 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.491$, $T_{max} = 0.551$	$k = -7 \rightarrow 13$
9422 measured reflections	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.121$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 2.5952P]$ where $P = (F_o^2 + 2F_c^2)/3$
6322 reflections	$(\Delta/\sigma)_{max} = 0.001$
415 parameters	$\Delta\rho_{max} = 1.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.70$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sn2	0.37891 (4)	0.50151 (4)	0.43671 (3)	0.03405 (14)

Sn1	0.52617 (4)	0.29250 (4)	0.32149 (3)	0.03909 (15)
O1	0.2765 (5)	0.2430 (7)	0.1747 (4)	0.108 (3)
Cl1	0.7318 (2)	0.0520 (2)	0.31794 (16)	0.0817 (7)
Cl3	0.1945 (2)	0.7643 (2)	0.47210 (16)	0.0889 (7)
O4	0.5297 (4)	0.4138 (3)	0.4439 (2)	0.0333 (9)
O3	0.3714 (4)	0.3739 (4)	0.3168 (3)	0.0457 (11)
H3	0.3230	0.3382	0.2763	0.069*
C24	0.1584 (6)	0.3003 (6)	0.4525 (5)	0.0455 (16)
C30	0.3829 (6)	0.6432 (6)	0.3587 (4)	0.0424 (15)
H30A	0.4072	0.7196	0.3957	0.051*
H30B	0.4431	0.6349	0.3122	0.051*
O2	0.4756 (5)	0.2118 (4)	0.1896 (3)	0.0555 (13)
C26	0.1527 (8)	0.0966 (8)	0.4741 (7)	0.077 (3)
H26	0.1734	0.0419	0.5092	0.093*
C20	0.4618 (10)	−0.1761 (7)	0.1799 (6)	0.077 (3)
H20	0.4560	−0.2425	0.1363	0.092*
C36	0.2531 (6)	0.6347 (6)	0.3195 (4)	0.0416 (15)
C2	0.3728 (9)	0.1342 (8)	0.0521 (5)	0.078 (3)
H2A	0.4492	0.1657	0.0250	0.094*
H2B	0.3766	0.0512	0.0559	0.094*
C32	0.0369 (8)	0.6721 (9)	0.3344 (7)	0.087 (3)
H32	−0.0233	0.7094	0.3661	0.104*
C23	0.1962 (6)	0.4311 (6)	0.4814 (5)	0.0479 (17)
H23A	0.1975	0.4470	0.5457	0.057*
H23B	0.1328	0.4728	0.4590	0.057*
C31	0.1583 (7)	0.6850 (7)	0.3675 (5)	0.059 (2)
C17	0.4781 (7)	0.0212 (6)	0.3103 (4)	0.0475 (17)
C18	0.5837 (7)	−0.0225 (6)	0.2777 (5)	0.0513 (18)
C1	0.3705 (8)	0.2012 (7)	0.1456 (5)	0.058 (2)
C16	0.4855 (7)	0.1312 (6)	0.3779 (4)	0.0505 (18)
H16A	0.5508	0.1298	0.4226	0.061*
H16B	0.4058	0.1304	0.4073	0.061*
C28	0.0522 (8)	0.1387 (11)	0.3465 (6)	0.089 (3)
H28	0.0067	0.1113	0.2932	0.107*
C25	0.1922 (7)	0.2164 (7)	0.4999 (5)	0.0556 (19)
C22	0.3625 (8)	−0.0376 (7)	0.2728 (5)	0.063 (2)
H22	0.2887	−0.0098	0.2917	0.075*
C35	0.2176 (8)	0.5672 (7)	0.2378 (5)	0.064 (2)
H35	0.2773	0.5319	0.2041	0.076*
C29	0.0866 (7)	0.2605 (8)	0.3724 (5)	0.067 (2)
H29	0.0628	0.3145	0.3378	0.081*
C19	0.5779 (9)	−0.1213 (7)	0.2139 (5)	0.068 (2)
H19	0.6511	−0.1498	0.1944	0.082*
C21	0.3545 (9)	−0.1354 (7)	0.2086 (6)	0.074 (3)
H21	0.2761	−0.1736	0.1849	0.089*
Cl4	0.2865 (2)	0.2618 (2)	0.59644 (16)	0.0855 (7)
Cl2	0.5677 (3)	0.5040 (3)	0.1524 (2)	0.1111 (10)
C15	0.8327 (7)	0.2995 (7)	0.1657 (5)	0.064 (2)
H15	0.8699	0.2630	0.2078	0.077*

C10	0.7379 (7)	0.3672 (6)	0.1912 (4)	0.0533 (19)
C9	0.7019 (6)	0.3859 (6)	0.2859 (4)	0.0531 (19)
H9A	0.7004	0.4704	0.3031	0.064*
H9B	0.7687	0.3647	0.3215	0.064*
C3	0.2613 (8)	0.1411 (7)	−0.0071 (4)	0.058 (2)
C11	0.6853 (8)	0.4162 (7)	0.1265 (5)	0.065 (2)
C14	0.8730 (9)	0.2849 (8)	0.0798 (7)	0.083 (3)
H14	0.9381	0.2412	0.0647	0.100*
C4	0.2413 (9)	0.2473 (8)	−0.0274 (6)	0.078 (3)
H4	0.2943	0.3160	−0.0024	0.093*
C27	0.0837 (9)	0.0588 (9)	0.3973 (8)	0.090 (3)
H27	0.0577	−0.0222	0.3794	0.108*
C13	0.8155 (11)	0.3359 (9)	0.0172 (6)	0.094 (4)
H13	0.8412	0.3257	−0.0410	0.112*
C8	0.1816 (11)	0.0414 (8)	−0.0418 (6)	0.099 (3)
H8	0.1937	−0.0325	−0.0279	0.119*
C7	0.0792 (11)	0.0515 (12)	−0.0997 (7)	0.106 (4)
H7	0.0231	−0.0159	−0.1231	0.127*
C12	0.7206 (10)	0.4017 (9)	0.0394 (6)	0.087 (3)
H12	0.6811	0.4357	−0.0032	0.104*
C34	0.0942 (10)	0.5521 (9)	0.2061 (7)	0.087 (3)
H34	0.0711	0.5061	0.1513	0.105*
C33	0.0056 (10)	0.6040 (11)	0.2544 (9)	0.103 (4)
H33	−0.0774	0.5925	0.2323	0.124*
C5	0.1443 (11)	0.2550 (11)	−0.0843 (7)	0.098 (3)
H5	0.1334	0.3291	−0.0985	0.118*
C6	0.0637 (10)	0.1576 (14)	−0.1206 (6)	0.101 (4)
H6	−0.0018	0.1643	−0.1595	0.121*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn2	0.0364 (2)	0.0383 (3)	0.0277 (2)	0.00952 (19)	−0.00245 (17)	0.00236 (18)
Sn1	0.0458 (3)	0.0380 (3)	0.0327 (3)	0.0095 (2)	0.00195 (19)	−0.00089 (19)
O1	0.050 (4)	0.200 (8)	0.062 (4)	0.038 (4)	−0.011 (3)	−0.038 (4)
Cl1	0.0591 (13)	0.0889 (17)	0.0930 (17)	0.0115 (11)	0.0016 (12)	−0.0006 (13)
Cl3	0.0980 (18)	0.0925 (18)	0.0805 (16)	0.0418 (14)	0.0156 (13)	−0.0022 (13)
O4	0.040 (2)	0.035 (2)	0.025 (2)	0.0114 (18)	−0.0045 (17)	0.0011 (17)
O3	0.046 (3)	0.049 (3)	0.038 (2)	0.014 (2)	−0.009 (2)	−0.012 (2)
C24	0.035 (4)	0.048 (4)	0.052 (4)	0.002 (3)	0.007 (3)	0.009 (3)
C30	0.043 (4)	0.046 (4)	0.041 (4)	0.013 (3)	0.000 (3)	0.011 (3)
O2	0.072 (3)	0.050 (3)	0.042 (3)	0.010 (3)	−0.007 (3)	−0.005 (2)
C26	0.071 (6)	0.062 (6)	0.104 (8)	0.009 (5)	0.025 (5)	0.025 (5)
C20	0.111 (8)	0.047 (5)	0.067 (6)	0.004 (5)	−0.004 (6)	−0.001 (4)
C36	0.046 (4)	0.039 (4)	0.042 (4)	0.003 (3)	−0.006 (3)	0.016 (3)
C2	0.106 (7)	0.085 (6)	0.041 (5)	0.029 (5)	−0.004 (4)	−0.011 (4)
C32	0.054 (5)	0.109 (8)	0.112 (8)	0.016 (5)	−0.001 (5)	0.061 (7)
C23	0.041 (4)	0.056 (4)	0.048 (4)	0.009 (3)	0.008 (3)	0.009 (3)

C31	0.047 (4)	0.065 (5)	0.074 (5)	0.014 (4)	−0.002 (4)	0.031 (4)
C17	0.059 (4)	0.038 (4)	0.048 (4)	0.008 (3)	0.006 (3)	0.011 (3)
C18	0.057 (4)	0.049 (4)	0.048 (4)	0.009 (3)	0.002 (3)	0.005 (3)
C1	0.075 (6)	0.056 (5)	0.036 (4)	0.004 (4)	−0.009 (4)	−0.005 (3)
C16	0.068 (5)	0.038 (4)	0.048 (4)	0.011 (3)	0.015 (4)	0.008 (3)
C28	0.067 (6)	0.115 (9)	0.064 (6)	−0.026 (6)	0.010 (5)	−0.022 (6)
C25	0.046 (4)	0.056 (5)	0.065 (5)	0.002 (4)	0.019 (4)	0.011 (4)
C22	0.062 (5)	0.054 (5)	0.073 (5)	0.008 (4)	0.006 (4)	0.011 (4)
C35	0.082 (6)	0.059 (5)	0.049 (5)	−0.002 (4)	−0.021 (4)	0.018 (4)
C29	0.055 (5)	0.077 (6)	0.063 (5)	−0.001 (4)	0.007 (4)	−0.002 (4)
C19	0.089 (6)	0.055 (5)	0.063 (5)	0.027 (5)	0.016 (5)	−0.001 (4)
C21	0.084 (7)	0.050 (5)	0.080 (6)	−0.012 (5)	−0.013 (5)	0.006 (4)
Cl4	0.0702 (14)	0.1108 (19)	0.0823 (16)	0.0166 (13)	−0.0149 (12)	0.0361 (14)
Cl2	0.127 (2)	0.114 (2)	0.118 (2)	0.0578 (18)	0.0473 (18)	0.0594 (18)
C15	0.070 (5)	0.051 (5)	0.070 (5)	0.011 (4)	0.019 (4)	0.002 (4)
C10	0.063 (5)	0.051 (4)	0.039 (4)	−0.011 (4)	0.015 (3)	−0.002 (3)
C9	0.051 (4)	0.057 (5)	0.043 (4)	−0.005 (3)	0.007 (3)	−0.005 (3)
C3	0.079 (5)	0.064 (5)	0.032 (4)	0.019 (4)	−0.001 (4)	−0.003 (3)
C11	0.081 (6)	0.053 (5)	0.061 (5)	0.010 (4)	0.019 (4)	0.010 (4)
C14	0.098 (7)	0.066 (6)	0.082 (7)	0.008 (5)	0.041 (6)	−0.003 (5)
C4	0.099 (7)	0.070 (6)	0.064 (6)	0.020 (5)	0.000 (5)	0.002 (5)
C27	0.079 (7)	0.064 (6)	0.115 (9)	−0.015 (5)	0.043 (7)	−0.007 (6)
C13	0.144 (10)	0.074 (7)	0.054 (6)	−0.007 (7)	0.045 (6)	−0.002 (5)
C8	0.150 (10)	0.058 (6)	0.080 (7)	−0.002 (6)	−0.030 (7)	0.004 (5)
C7	0.114 (9)	0.111 (10)	0.077 (7)	−0.010 (7)	−0.028 (6)	−0.010 (7)
C12	0.119 (8)	0.088 (7)	0.053 (5)	0.009 (6)	0.018 (5)	0.015 (5)
C34	0.092 (7)	0.085 (7)	0.078 (7)	−0.024 (6)	−0.039 (6)	0.034 (5)
C33	0.058 (6)	0.125 (10)	0.130 (10)	−0.024 (6)	−0.039 (7)	0.077 (8)
C5	0.116 (9)	0.121 (10)	0.071 (7)	0.053 (7)	−0.007 (6)	0.024 (6)
C6	0.089 (8)	0.160 (12)	0.055 (6)	0.037 (8)	−0.008 (5)	0.006 (7)

Geometric parameters (Å, °)

Sn1—O3	2.023 (4)	C18—C19	1.377 (10)
Sn1—O2	2.114 (4)	C16—H16A	0.9700
Sn1—C9	2.145 (6)	C16—H16B	0.9700
Sn1—C16	2.145 (7)	C28—C27	1.356 (14)
Sn1—O4	2.157 (3)	C28—C29	1.390 (12)
Sn2—O4	2.033 (4)	C28—H28	0.9300
Sn2—O4^{i}	2.089 (3)	C25—Cl4	1.740 (8)
Sn2—C30	2.146 (6)	C22—C21	1.369 (11)
Sn2—O3	2.163 (4)	C22—H22	0.9300
Sn2—C23	2.165 (6)	C35—C34	1.377 (11)
Sn2—Sn2^{i}	3.2130 (8)	C35—H35	0.9300
O1—C1	1.238 (9)	C29—H29	0.9300
Cl1—C18	1.745 (7)	C19—H19	0.9300
Cl3—C31	1.725 (8)	C21—H21	0.9300
O4—Sn2^{i}	2.089 (3)	Cl2—C11	1.741 (8)

O3—H3	0.8200	C15—C14	1.379 (11)
C24—C25	1.370 (10)	C15—C10	1.395 (10)
C24—C29	1.412 (10)	C15—H15	0.9300
C24—C23	1.496 (9)	C10—C11	1.357 (11)
C30—C36	1.487 (8)	C10—C9	1.494 (9)
C30—H30A	0.9700	C9—H9A	0.9700
C30—H30B	0.9700	C9—H9B	0.9700
O2—C1	1.281 (8)	C3—C4	1.346 (11)
C26—C27	1.355 (13)	C3—C8	1.357 (11)
C26—C25	1.377 (11)	C11—C12	1.380 (11)
C26—H26	0.9300	C14—C13	1.371 (14)
C20—C21	1.359 (12)	C14—H14	0.9300
C20—C19	1.366 (11)	C4—C5	1.362 (12)
C20—H20	0.9300	C4—H4	0.9300
C36—C35	1.384 (9)	C27—H27	0.9300
C36—C31	1.405 (10)	C13—C12	1.371 (14)
C2—C3	1.503 (11)	C13—H13	0.9300
C2—C1	1.521 (9)	C8—C7	1.425 (14)
C2—H2A	0.9700	C8—H8	0.9300
C2—H2B	0.9700	C7—C6	1.335 (15)
C32—C33	1.358 (14)	C7—H7	0.9300
C32—C31	1.366 (11)	C12—H12	0.9300
C32—H32	0.9300	C34—C33	1.364 (15)
C23—H23A	0.9700	C34—H34	0.9300
C23—H23B	0.9700	C33—H33	0.9300
C17—C18	1.374 (9)	C5—C6	1.352 (14)
C17—C22	1.392 (10)	C5—H5	0.9300
C17—C16	1.502 (9)	C6—H6	0.9300

O4—Sn2—O4^{i}	77.61 (16)	C17—C16—H16A	109.0
O4—Sn2—C30	120.9 (2)	Sn1—C16—H16A	109.0
O4^{i}—Sn2—C30	103.2 (2)	C17—C16—H16B	109.0
O4—Sn2—O3	72.95 (15)	Sn1—C16—H16B	109.0
O4^{i}—Sn2—O3	150.47 (16)	H16A—C16—H16B	107.8
C30—Sn2—O3	90.1 (2)	C27—C28—C29	121.5 (9)
O4—Sn2—C23	121.1 (2)	C27—C28—H28	119.3
O4^{i}—Sn2—C23	101.5 (2)	C29—C28—H28	119.3
C30—Sn2—C23	116.6 (3)	C24—C25—C26	121.9 (8)
O3—Sn2—C23	95.6 (2)	C24—C25—Cl4	119.4 (6)
O4—Sn2—Sn2^{i}	39.43 (10)	C26—C25—Cl4	118.7 (7)
O4^{i}—Sn2—Sn2^{i}	38.18 (11)	C21—C22—C17	121.7 (8)
C30—Sn2—Sn2^{i}	118.26 (17)	C21—C22—H22	119.2
O3—Sn2—Sn2^{i}	112.35 (11)	C17—C22—H22	119.2
C23—Sn2—Sn2^{i}	117.14 (19)	C34—C35—C36	120.4 (9)
O3—Sn1—O2	86.93 (17)	C34—C35—H35	119.8
O3—Sn1—C9	117.5 (3)	C36—C35—H35	119.8
O2—Sn1—C9	93.6 (2)	C28—C29—C24	118.5 (9)
O3—Sn1—C16	111.2 (2)	C28—C29—H29	120.8

O2—Sn1—C16	95.2 (2)	C24—C29—H29	120.8
C9—Sn1—C16	130.8 (3)	C20—C19—C18	118.2 (8)
O3—Sn1—O4	73.29 (15)	C20—C19—H19	120.9
O2—Sn1—O4	159.50 (18)	C18—C19—H19	120.9
C9—Sn1—O4	90.9 (2)	C20—C21—C22	119.6 (8)
C16—Sn1—O4	96.9 (2)	C20—C21—H21	120.2
Sn2—O4—Sn2^{i}	102.39 (16)	C22—C21—H21	120.2
Sn2—O4—Sn1	106.75 (16)	C14—C15—C10	122.0 (9)
Sn2^{i}—O4—Sn1	150.5 (2)	C14—C15—H15	119.0
Sn1—O3—Sn2	106.89 (18)	C10—C15—H15	119.0
Sn1—O3—H3	109.5	C11—C10—C15	116.4 (7)
Sn2—O3—H3	142.1	C11—C10—C9	123.4 (7)
C25—C24—C29	118.0 (7)	C15—C10—C9	120.2 (8)
C25—C24—C23	122.7 (6)	C10—C9—Sn1	118.6 (4)
C29—C24—C23	119.2 (7)	C10—C9—H9A	107.7
C36—C30—Sn2	106.7 (4)	Sn1—C9—H9A	107.7
C36—C30—H30A	110.4	C10—C9—H9B	107.7
Sn2—C30—H30A	110.4	Sn1—C9—H9B	107.7
C36—C30—H30B	110.4	H9A—C9—H9B	107.1
Sn2—C30—H30B	110.4	C4—C3—C8	119.5 (9)
H30A—C30—H30B	108.6	C4—C3—C2	119.6 (8)
C1—O2—Sn1	129.9 (5)	C8—C3—C2	120.9 (8)
C27—C26—C25	119.8 (9)	C10—C11—C12	123.5 (8)
C27—C26—H26	120.1	C10—C11—Cl2	119.6 (6)
C25—C26—H26	120.1	C12—C11—Cl2	116.8 (8)
C21—C20—C19	121.2 (8)	C13—C14—C15	118.9 (9)
C21—C20—H20	119.4	C13—C14—H14	120.5
C19—C20—H20	119.4	C15—C14—H14	120.5
C35—C36—C31	117.1 (7)	C3—C4—C5	120.6 (9)
C35—C36—C30	121.3 (7)	C3—C4—H4	119.7
C31—C36—C30	121.4 (6)	C5—C4—H4	119.7
C3—C2—C1	114.5 (7)	C26—C27—C28	120.2 (9)
C3—C2—H2A	108.6	C26—C27—H27	119.9
C1—C2—H2A	108.6	C28—C27—H27	119.9
C3—C2—H2B	108.6	C12—C13—C14	120.8 (8)
C1—C2—H2B	108.6	C12—C13—H13	119.6
H2A—C2—H2B	107.6	C14—C13—H13	119.6
C33—C32—C31	118.9 (10)	C3—C8—C7	119.1 (10)
C33—C32—H32	120.5	C3—C8—H8	120.5
C31—C32—H32	120.5	C7—C8—H8	120.5
C24—C23—Sn2	114.0 (4)	C6—C7—C8	120.2 (10)
C24—C23—H23A	108.8	C6—C7—H7	119.9
Sn2—C23—H23A	108.8	C8—C7—H7	119.9
C24—C23—H23B	108.8	C13—C12—C11	118.4 (10)
Sn2—C23—H23B	108.8	C13—C12—H12	120.8
H23A—C23—H23B	107.7	C11—C12—H12	120.8
C32—C31—C36	122.1 (8)	C33—C34—C35	120.6 (9)
C32—C31—Cl3	118.4 (7)	C33—C34—H34	119.7

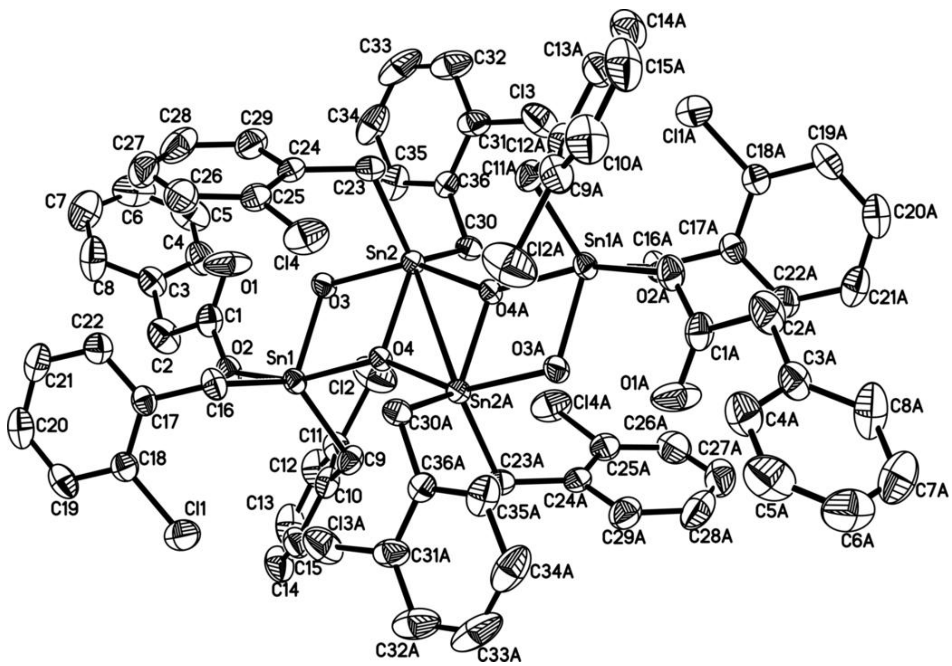
C36—C31—Cl3	119.5 (5)	C35—C34—H34	119.7
C18—C17—C22	116.3 (6)	C32—C33—C34	120.9 (9)
C18—C17—C16	122.6 (6)	C32—C33—H33	119.5
C22—C17—C16	121.0 (7)	C34—C33—H33	119.5
C17—C18—C19	123.1 (7)	C6—C5—C4	121.5 (11)
C17—C18—Cl1	118.5 (5)	C6—C5—H5	119.2
C19—C18—Cl1	118.5 (6)	C4—C5—H5	119.2
O1—C1—O2	124.1 (6)	C7—C6—C5	119.1 (11)
O1—C1—C2	122.6 (7)	C7—C6—H6	120.5
O2—C1—C2	113.2 (7)	C5—C6—H6	120.5
C17—C16—Sn1	113.0 (5)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.82	1.78	2.554 (7)	157.

Fig. 1


C14A
C13A
C15A
C33
C32
C13
C34
C28
C29
Cl1A
C19A
C27
C24
C31
C12A
C35
C10A
C18A
C11A
C23
C36
C26
C9A
C7
C6
C25
C5
C30
Sn1A
C16A
C17A
C20A
C4
Cl4
Sn2
Cl2A
O1
C8
C3
O2A
C22A
O3
O4A
C21A
C2A
C1
C22
O2
Sn1
O4
O3A
C1A
C3A
C2
Cl2
C21
Sn2A
Cl4A
O1A
C8A
C16
C17
C30A
C26A
C4A
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C11
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C27A
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C36A
C23A
C25A
C18
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C19
Cl1
C24A
C5A
C13
C35A
Cl3A
C29A
C28A
C6A
C15
C31A
C14
C34A
C32A
C33A