

# Octakis(2-chlorobenzyl)di- $\mu_2$ -hydroxido-di- $\mu_3$ -oxido-bis(2-phenylacetato)tetra-tin(IV)

Wei-Bing Peng,<sup>a</sup> Guo-Qiang Li,<sup>a</sup> Handong Yin<sup>b\*</sup> and Xianhe Zhao<sup>b</sup>

<sup>a</sup>Key Laboratory of Marine Drugs, Chinese Ministry of Education, Marine Drug and Food Institute, Ocean University of China, Qingdao 266003, People's Republic of China, and <sup>b</sup>College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China  
Correspondence e-mail: guoqiangliouc@163.com

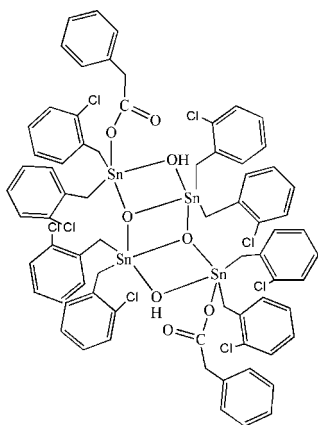
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.013$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.121; data-to-parameter ratio = 15.2.

The asymmetric unit of the title compound,  $[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8(\text{C}_8\text{H}_7\text{O}_2)_2\text{O}_2(\text{OH})_2]$ , comprises one-half of the centrosymmetric tin(IV) complex.  $\mu_3$ -Oxide and  $\mu_2$ -hydroxide bridges link the four five-coordinate  $\text{Sn}^{\text{IV}}$  atoms to generate three fused four-membered  $\text{Sn}-\text{O}-\text{Sn}-\text{O}$  rings in a ladder-like structure. The two endocyclic Sn atoms each bind to two  $\mu_3$ -oxide anions and a  $\mu_2$ -hydroxide ligand, together with two 2-chlorobenzyl groups. The exocyclic Sn atoms each carry a monodentate phenylacetate ligand, two 2-chlorobenzyl groups, and  $\mu_3$ -oxide and  $\mu_2$ -hydroxide ligands. Both types of Sn atoms adopt a distorted trigonal-bipyramidal coordination geometry. The molecular conformation is stabilized by intramolecular  $\text{O}-\text{H}\cdots\text{O}$  interactions involving the  $\mu_2$ -hydroxide ligands and the  $\text{C}=\text{O}$  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

$[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8(\text{C}_8\text{H}_7\text{O}_2)_2\text{O}_2(\text{OH})_2]$	$\gamma = 98.404$ (2) $^\circ$
$M_r = 1815.59$	$V = 1833.6$ (4) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 1$
$a = 10.7095$ (14) Å	Mo $K\alpha$ radiation
$b = 11.4846$ (16) Å	$\mu = 1.69$ mm <sup>-1</sup>
$c = 15.2412$ (18) Å	$T = 298$ K
$\alpha = 98.311$ (2) $^\circ$	$0.49 \times 0.48 \times 0.40$ mm
$\beta = 90.982$ (1) $^\circ$	

### Data collection

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

### Refinement

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

**Table 1**

Selected bond lengths (Å).

Sn1—O3	2.023 (4)	Sn2—O4	2.033 (4)
Sn1—O2	2.114 (4)	Sn2—O4 <sup>i</sup>	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,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O3—H3 $\cdots$ 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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Wu, X., Kang, W., Zhu, D., Zhu, C. & Liu, S. (2009). *J. Organomet. Chem.* **694**, 2981–2986.

## supporting information

*Acta Cryst.* (2010). E66, m535–m536 [https://doi.org/10.1107/S1600536810012559]

**Octakis(2-chlorobenzyl)di- $\mu_2$ -hydroxido-di- $\mu_3$ -oxido-bis(2-phenylacetato)-tetratin(IV)****Wei-Bing Peng, Guo-Qiang Li, Handong Yin and Xianhe Zhao****S1. 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  $\mu_3$ -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  $\mu_2$ -hydroxide anions and  $\mu_3$ -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 $\cdots$ O1 hydrogen bonds (Table 2). The crystal structure of a similar compound has been reported recently (Wu *et al.*, 2009).

**S2. 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).

**S3. 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  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  or  $1.5 U_{\text{eq}}(\text{O})$  for hydroxyl groups

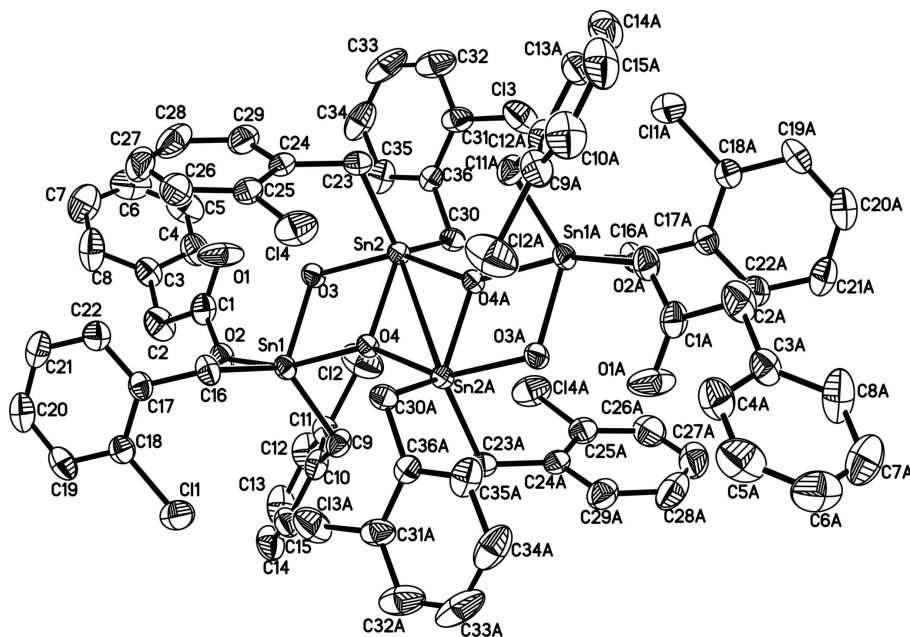


Figure 1

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

#### Octakis(2-chlorobenzyl)di- $\mu_2$ -hydroxido-di- $\mu_3$ -oxido-bis(2-phenylacetato)tetratin(IV)

##### Crystal data

$[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8(\text{C}_8\text{H}_7\text{O}_2)_2\text{O}_2(\text{OH})_2]$

$M_r = 1815.59$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 10.7095$  (14) Å

$b = 11.4846$  (16) Å

$c = 15.2412$  (18) Å

$\alpha = 98.311$  (2)°

$\beta = 90.982$  (1)°

$\gamma = 98.404$  (2)°

$V = 1833.6$  (4) Å<sup>3</sup>

$Z = 1$

$F(000) = 896$

$D_x = 1.644$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4098 reflections

$\theta = 2.3\text{--}27.0^\circ$

$\mu = 1.69$  mm<sup>-1</sup>

$T = 298$  K

Block, colourless

$0.49 \times 0.48 \times 0.40$  mm

##### Data collection

Siemens SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.491$ ,  $T_{\max} = 0.551$

9422 measured reflections

6322 independent reflections

4437 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 1.4^\circ$

$h = -12 \rightarrow 12$

$k = -7 \rightarrow 13$

$l = -18 \rightarrow 17$

##### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.121$

$S = 1.05$

6322 reflections

415 parameters

0 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 2.5952P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.18 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)

C13	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)
C14	0.0702 (14)	0.1108 (19)	0.0823 (16)	0.0166 (13)	-0.0149 (12)	0.0361 (14)
C12	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 <sup>i</sup>	2.089 (3)	C25—C14	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 <sup>i</sup>	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 <sup>i</sup>	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 <sup>i</sup>	77.61 (16)	C17—C16—H16A	109.0
O4—Sn2—C30	120.9 (2)	Sn1—C16—H16A	109.0
O4 <sup>i</sup> —Sn2—C30	103.2 (2)	C17—C16—H16B	109.0
O4—Sn2—O3	72.95 (15)	Sn1—C16—H16B	109.0
O4 <sup>i</sup> —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 <sup>i</sup> —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—C14	119.4 (6)
O4—Sn2—Sn2 <sup>i</sup>	39.43 (10)	C26—C25—C14	118.7 (7)
O4 <sup>i</sup> —Sn2—Sn2 <sup>i</sup>	38.18 (11)	C21—C22—C17	121.7 (8)
C30—Sn2—Sn2 <sup>i</sup>	118.26 (17)	C21—C22—H22	119.2
O3—Sn2—Sn2 <sup>i</sup>	112.35 (11)	C17—C22—H22	119.2
C23—Sn2—Sn2 <sup>i</sup>	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 <sup>i</sup>	102.39 (16)	C22—C21—H21	120.2
Sn2—O4—Sn1	106.75 (16)	C14—C15—C10	122.0 (9)
Sn2 <sup>i</sup> —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—C12	119.6 (6)
C25—C26—H26	120.1	C12—C11—C12	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 code: (i)  $-x+1, -y+1, -z+1$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3 $\cdots$ O1	0.82	1.78	2.554 (7)	157