

Fa-Hui Li, Han-Dong Yin,\*  
Wen-Bo Huang and Yu-Wei  
WangCollege of Chemistry and Chemical Engineering,  
Liaocheng University, Shandong 252059,  
People's Republic of China

Correspondence e-mail: yinhandong@tom.com

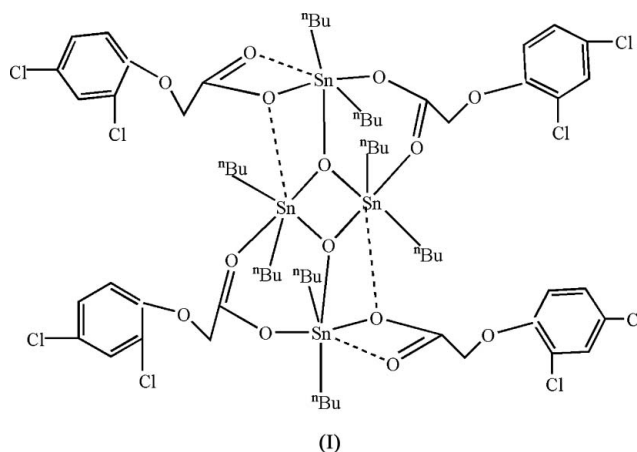
## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.016$  Å  
Disorder in main residue  
 $R$  factor = 0.049  
 $wR$  factor = 0.134  
Data-to-parameter ratio = 15.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Octabutyl- $1\kappa^2\text{C}, 2\kappa^2\text{C}, 3\kappa^2\text{C}, 4\kappa^2\text{C}$ -bis( $\mu_2$ -2,4-dichloro-  
phenoxyacetato)- $1:2\kappa^2\text{O}:O'; 3:4\kappa^2\text{O}:O'$ -bis(2,4-  
dichlorophenoxyacetato)- $1\kappa\text{O}, 4\kappa\text{O}$ -di- $\mu_3$ -oxo-  
 $1:2:3\kappa^3\text{O}:O:O; 2:3:4\kappa^3\text{O}:O:O$ -tetratin(IV)The title compound,  $[\text{Sn}_4(\text{C}_4\text{H}_9)_8(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_3)_4\text{O}_2]$ , is a cluster built up by inversion symmetry around the central  $\text{Sn}_2\text{O}_2$  ring. Both unique  $\text{SnO}_3\text{C}_2$  centres have a distorted trigonal-bipyramidal geometry with the O atoms in axial positions.

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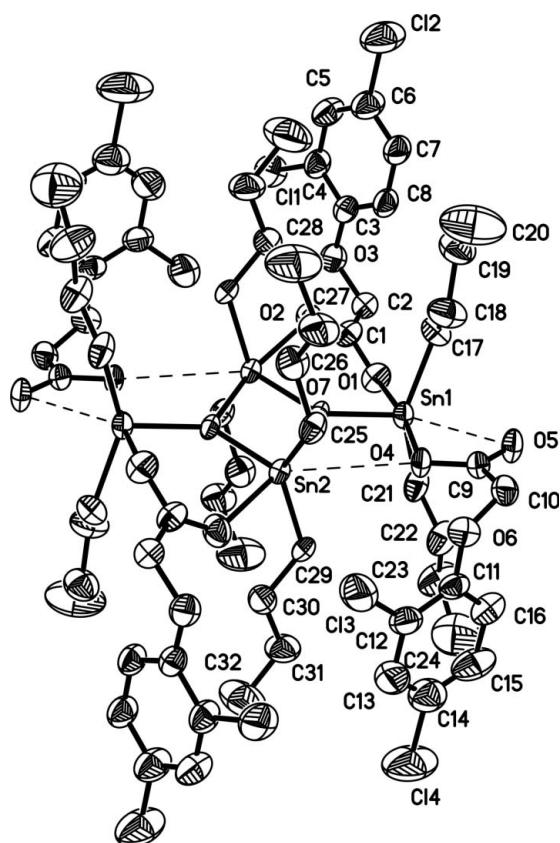
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## Comment

The title compound, (I) (Fig. 1), is a cluster containing four Sn atoms. The whole molecule lies about a centre of symmetry with a central  $\text{Sn}_2\text{O}_2$  core and the structure is similar to those seen previously in related compounds (Yin *et al.*, 2003). The three-coordinate  $\mu_3$ -bridging atom O7 in the  $\text{Sn}_2\text{O}_2$  ring is also attached to a  $\text{Bu}_2\text{SnO}_2$  unit. Moreover, the C1 carboxylate group coordinates to each Sn atom in a bridging mode (Fig. 2).

The geometry at both the independent Sn atoms is distorted trigonal-bipyramidal (Table 1). The exocyclic atoms bonded to Sn1, *viz.* O1 and O4 are in axial positions [ $\text{O1}-\text{Sn1}-\text{O4} = 171.7(2)^\circ$ ], and the C atoms of the two butyl groups and O7 are in equatorial positions. The r.m.s. deviation from the O7/Sn1/C17/C21 mean plane is 0.0776 Å. The geometry of the Sn2 atom in the  $\text{Sn}_2\text{O}_2$  ring is slightly different from that of Sn1. Here, atoms O2<sup>i</sup> [symmetry code: (i)  $-x + 1, -y + 1, -z$ ] and O7 are in axial positions with  $\text{O7}-\text{Sn2}-\text{O2}^i = 166.97(19)^\circ$ , and the C atoms of the two butyl groups and O7<sup>i</sup> are equatorial. The r.m.s. deviation from the O7<sup>i</sup>/Sn2/C25/C29 mean plane is 0.0093 Å, indicating a greater degree of planarity.

The severe distortion from trigonal-planar geometry in the equatorial planes, signalled by the individual C-Sn-C and C-Sn-O angles at both Sn atoms, is clearly also related to the relatively short Sn1 $\cdots$ O5 and Sn2 $\cdots$ O4 contacts. At 2.806(5) and 3.182(4) Å, respectively, these are much shorter than the sum of the van der Waals radii (4.0 Å; Vollano *et al.*, 1984).


**Figure 1**

The molecular structure of (I), with 30% probability displacement ellipsoids (H atoms have been omitted for clarity). The unlabelled atoms are generated by the symmetry operation  $(-x + 1, -y + 1, -z)$ . Short Sn1...O5 and Sn2...O4 contacts are displayed as dashed lines

## Experimental

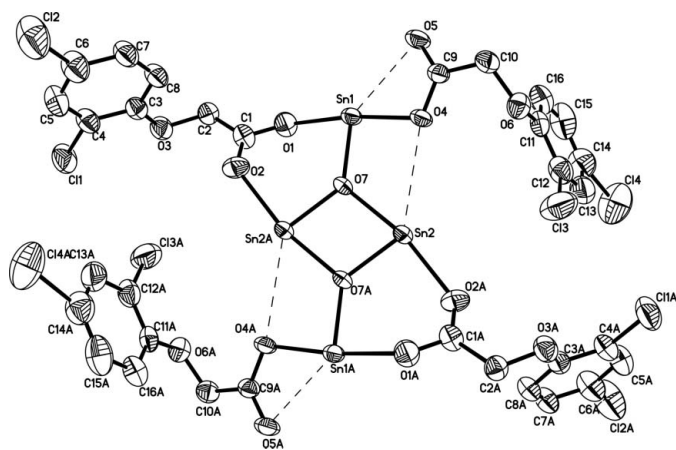
A mixture of dibutyltin oxide (0.4978 g, 2.0 mmol) and 2,4-dichlorophenoxyacetic acid (0.4421 g, 2.0 mmol) in methanol (80 ml) was heated under reflux for 8 h. The solvent was removed under vacuum and the product crystallized from a mixture of dichloromethane/ethanol (1:1) to yield colourless blocks of (I) (0.6361 g, 69%; m.p. 416 K). Analysis calculated for  $C_{64}H_{92}Cl_8O_{14}Sn_4$ : C 41.69, H 5.03%; found: C 41.73, H 5.06%.

### Crystal data

$[Sn_4(C_4H_9)_8(C_8H_5Cl_2O_3)_4O_2]$	$Z = 1$
$M_r = 1843.74$	$D_x = 1.581 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 12.020 (3) \text{ \AA}$	Cell parameters from 3064 reflections
$b = 12.488 (3) \text{ \AA}$	$\theta = 2.3\text{--}23.2^\circ$
$c = 14.562 (3) \text{ \AA}$	$\mu = 1.61 \text{ mm}^{-1}$
$\alpha = 88.964 (3)^\circ$	$T = 298 (2) \text{ K}$
$\beta = 84.890 (3)^\circ$	Block, colourless
$\gamma = 62.852 (3)^\circ$	$0.52 \times 0.41 \times 0.39 \text{ mm}$
$V = 1936.5 (7) \text{ \AA}^3$	

### Data collection

Bruker SMART CCD area-detector diffractometer	6751 independent reflections
$\varphi$ and $\omega$ scans	4330 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$R_{int} = 0.029$
$T_{min} = 0.456, T_{max} = 0.534$	$\theta_{max} = 25.0^\circ$
10200 measured reflections	$h = -14 \rightarrow 14$
	$k = -14 \rightarrow 14$
	$l = -14 \rightarrow 17$


**Figure 2**

In this view the *n*-butyl groups have been omitted for clarity. Atoms with the suffix *A* are generated by the symmetry operation  $(-x + 1, -y + 1, -z)$ . Short Sn1...O5 and Sn2...O4 contacts are displayed as dashed lines

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.134$   
 $S = 1.00$   
 6751 reflections  
 426 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 5.3146P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{max} < 0.001$$

$$\Delta\rho_{max} = 1.79 \text{ e \AA}^{-3}$$

$$\Delta\rho_{min} = -0.68 \text{ e \AA}^{-3}$$

**Table 1**

Selected geometric parameters ( $\text{\AA}, ^\circ$ ).

Sn1—O7	2.033 (4)	Sn2—C25	2.125 (7)
Sn1—C17	2.122 (8)	Sn2—O7	2.197 (5)
Sn1—O4	2.157 (5)	Sn2—O2 <sup>i</sup>	2.275 (5)
Sn1—C21	2.171 (9)	Sn2—O4	3.182 (4)
Sn1—O1	2.284 (6)	O1—C1	1.272 (9)
Sn1—O5	2.806 (5)	O2—C1	1.232 (9)
Sn2—O7 <sup>i</sup>	2.027 (4)	O4—C9	1.281 (8)
Sn2—C29	2.120 (7)	O5—C9	1.216 (8)
O7—Sn1—C17	103.9 (3)	C29—Sn2—C25	133.5 (3)
O7—Sn1—O4	84.40 (17)	O7 <sup>i</sup> —Sn2—O7	75.75 (18)
C17—Sn1—O4	100.4 (3)	C29—Sn2—O7	93.9 (3)
O7—Sn1—C21	111.0 (3)	C25—Sn2—O7	99.2 (3)
C17—Sn1—C21	141.9 (4)	O7 <sup>i</sup> —Sn2—O2 <sup>i</sup>	92.0 (2)
O4—Sn1—C21	97.8 (3)	C29—Sn2—O2 <sup>i</sup>	87.2 (3)
O7—Sn1—O1	90.83 (19)	C25—Sn2—O2 <sup>i</sup>	89.4 (3)
C17—Sn1—O1	87.4 (3)	O7—Sn2—O2 <sup>i</sup>	166.97 (19)
O4—Sn1—O1	171.7 (2)	O7 <sup>i</sup> —Sn2—O4	135.20 (15)
C21—Sn1—O1	77.5 (3)	C29—Sn2—O4	76.1 (2)
O7—Sn1—O5	134.08 (17)	C25—Sn2—O4	72.7 (2)
C17—Sn1—O5	79.4 (3)	O7—Sn2—O4	59.87 (14)
O4—Sn1—O5	50.61 (16)	O2 <sup>i</sup> —Sn2—O4	132.70 (18)
C21—Sn1—O5	86.9 (3)	Sn2 <sup>i</sup> —O7—Sn1	129.6 (2)
O1—Sn1—O5	134.96 (19)	Sn2 <sup>i</sup> —O7—Sn2	104.25 (18)
O7 <sup>i</sup> —Sn2—C29	115.1 (3)	Sn1—O7—Sn2	125.6 (2)
O7 <sup>i</sup> —Sn2—C25	111.4 (2)		

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

Atoms C14, C19 and C20 were disordered over two positions. Final site occupancy factors were 0.63 (3) and 0.37 (3) for C14, and 0.73 (4) and 0.27 (4) for C19 and C20. H atoms were positioned geometrically [ $C-H = 0.93$  (CH),  $0.97$  (CH<sub>2</sub>) and  $0.96 \text{ \AA}$  (CH<sub>3</sub>)] and constrained to ride on their parent atoms with  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(\text{methyl } C)$ . The highest density peak is located  $0.92 \text{ \AA}$  from atom Sn1.

Data collection: *SMART* (Bruker 1998); cell refinement: *SAINTE* (Bruker 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 1998); software used to prepare material for publication: *SHELXTL*.

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