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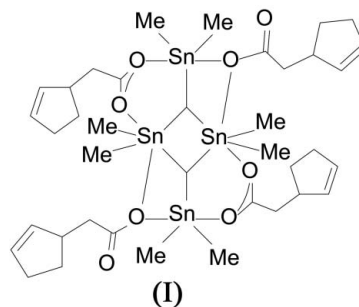
## Key indicators

Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
Disorder in main residue  
 $R$  factor = 0.036  
 $wR$  factor = 0.084  
Data-to-parameter ratio = 21.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(cyclopentenylacetato)tetramethyl-  
distannoxane dimer

The crystal structure of the title compound, tetra- $\mu_2$ -(cyclopent-2-enyl)acetato-1:2 $\kappa^2$ O:O';1:3 $\kappa^2$ O:O';2:4 $\kappa^2$ O:O';-3:4 $\kappa^2$ O:O'-octamethyl-1 $\kappa^2$ C,2 $\kappa^2$ C,3 $\kappa^2$ C,4 $\kappa^2$ C-di- $\mu_3$ -oxo-1:2:3 $\kappa^3$ O;2:3:4 $\kappa^3$ O-tetratin(IV),  $[\text{Sn}_4(\text{CH}_3)_8(\text{C}_7\text{H}_9\text{O}_2)_4\text{O}_2]$ , is composed of discrete centrosymmetric dimers lying about inversion centres. The cyclopentenylacetate ligand shows different modes of coordination with Sn, as a result of which the central  $\text{Sn}_2\text{O}_2$  core is fused with two four-membered ( $\text{Sn}_2\text{O}_2$ ) and two six-membered ( $\text{Sn}_2\text{O}_3\text{C}$ ) rings. The endocyclic Sn atoms are six-coordinate in a skew-trapezoidal bipyramidal environment. The exocyclic Sn atoms are five-coordinate and show distorted trigonal-bipyramidal geometry. The Sn—C distances lie in a very narrow range [2.095 (4)–2.113 (4) Å], while the Sn—O distances range between 2.030 (3) and 2.280 (3) Å for strong bonds and a value of 2.654 (3) Å for the relatively weak Sn—O bond.

## Comment

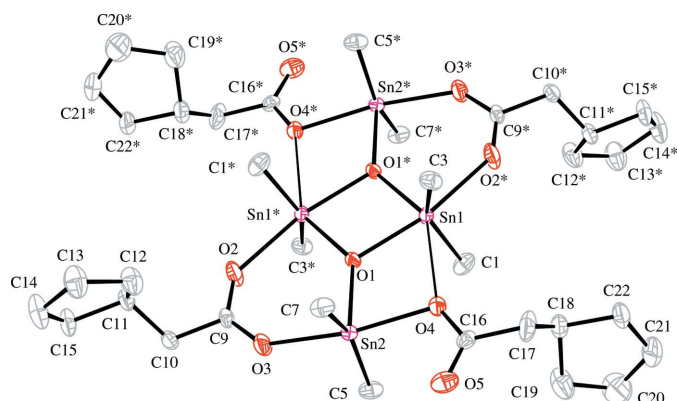
Organotin compounds have important applications in the chemical industry. They are used in the stabilization of PVC to prevent thermal degradation during processing and long-term photodegradation (Ahmad *et al.*, 2000). They are widely employed as catalysts (Al-Allaf *et al.*, 1999), as well as effective antitumour agents (Davies & Smith, 1982). The structural aspects of several organotin carboxylates have been reported from our laboratories (Parvez, Ali, Mazhar, Bhatti & Khokhar, 1999; Parvez, Ali, Bhatti *et al.*, 1999; Parvez, Ali, Mazhar, Bhatti & Choudhary, 1999; Parvez *et al.*, 2000, 2002; Sadiq-ur-Rehman, Shouldice *et al.*, 2004; Sadiq-ur-Rehman, Abdelrahman *et al.*, 2004). We have now synthesized a new compound, the tetramethylbis(cyclopentenylacetato)distannoxane dimer, (I), the structure of which is reported here.



The structure of (I) is composed of centrosymmetric dimers lying about inversion centres (Fig. 1). The cyclopentenylacetate ligand shows different modes of coordination with Sn. It acts as a monodentate ligand, bridging two Sn atoms *via* atom O4 to form a four-membered ring, Sn1/O4/Sn2/O1. The ligand also bridges two Sn atoms in bidentate coordination,

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**Figure 1**

A drawing of a dimer of (I), with displacement ellipsoids plotted at the 30% probability level. H atoms and the minor component of the disorder have been omitted for clarity. [Symmetry code: \*  $-x, 1 - y, 1 - z$ .]

thus resulting in a six-membered ring, Sn1<sup>i</sup>/O1/Sn2/O3/C9/O2 [symmetry code: (i)  $-x, -y + 1, -z + 1$ ]. As a result, the central Sn<sub>2</sub>O<sub>2</sub> core is fused with two four-membered (Sn<sub>2</sub>O<sub>2</sub>) and two six-membered (Sn<sub>2</sub>O<sub>3</sub>C) rings. The geometry around the six-coordinate endocyclic Sn atoms is skew-trapezoidal bipyramidal, while in the five-coordinate exocyclic Sn atoms it is distorted trigonal-bipyramidal.

The Sn—C distances lie in a very narrow range of 2.095 (4)–2.113 (4) Å, while the Sn—O distances range between 2.030 (3) and 2.280 (3) Å for strong bonds and have a value of 2.654 (3) Å for the relatively weak Sn—O bond. The endocyclic Sn—O distances in the central Sn1/O1/Sn1<sup>i</sup>/O1<sup>i</sup> core [2.030 (3) and 2.128 (3) Å] and the exocyclic Sn1—O2<sup>i</sup> distance [2.280 (3) Å] are similar to those observed in bis[1,1,3,3-tetrabutyl-1,3-bis(picolinato *N*-oxide)]distannoxane hydrate (Ng, 1998), tetrabutylbis(*N*-phthaloylglycinato)-distannoxane dimer (Parvez *et al.*, 2000), tetrabutylbis(*N*-phthaloylphenylalaninato)-distannoxane dimer (Hans *et al.*, 2002) and bis(cyclopentenylacetato)tetraethyl-distannoxane dimer (Ahmad *et al.*, 2006). However, the Sn1···O4<sup>i</sup> interaction [2.654 (3) Å] in (I) is significantly shorter than the corresponding interactions observed in tetrabutylbis(*N*-phthaloylphenylalaninato)-distannoxane dimer [2.725 (3) Å; Hans *et al.*, 2002] and tetrabutylbis(*N*-phthaloylglycinato)-distannoxane dimer [2.746 (3) Å; Parvez *et al.*, 2000]. A search of the Cambridge Structural Database (2006 Release; Allen, 2002) for similar fused-ring systems resulted in 80 hits, 16 of which contained dimethyltin units.

As observed in the similar structures quoted above, one of the ligands is coordinated to both Sn atoms, with C—O distances lying in between a single and a double bond, representing a delocalized system. In the other ligand, the O—C distances clearly indicate a single and a double bond (details in Table 1).

## Experimental

A mixture of dimethyltin(IV) oxide (1.50 g, 6.63 mmol) and 2-(cyclopentenyl)acetic acid (1.72 g, 13.26 mmol), in a 250 ml two-

necked round-bottomed flask fitted with a water condenser and magnet bar, was refluxed with constant stirring in dry toluene (100 ml) for 8 h in the presence of triethylamine (1.43 g, 13.86 mmol). The reaction mixture was then cooled to room temperature and the solid Et<sub>3</sub>NHCl salt which had formed was removed by filtration. The solvent was evaporated on a rotary evaporator and the liquid product thus obtained was purified *via* vacuum distillation. Crystals of (I) suitable for single-crystal X-ray analysis were grown by placing the liquid product in a glass vial for several weeks without the addition of any solvent.

## Crystal data

[Sn<sub>4</sub>(CH<sub>3</sub>)<sub>8</sub>(C<sub>7</sub>H<sub>9</sub>O<sub>2</sub>)<sub>4</sub>O<sub>2</sub>]  
*M<sub>r</sub>* = 1127.60  
 Triclinic, *P* $\bar{1}$   
*a* = 7.572 (2) Å  
*b* = 11.154 (3) Å  
*c* = 13.387 (4) Å  
 $\alpha$  = 84.584 (9)°  
 $\beta$  = 76.014 (9)°  
 $\gamma$  = 89.404 (15)°

*V* = 1092.1 (5) Å<sup>3</sup>  
*Z* = 1  
*D<sub>x</sub>* = 1.714 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 2.31 mm<sup>-1</sup>  
*T* = 173 (2) K  
 Prism, colourless  
 0.10 × 0.09 × 0.08 mm

## Data collection

Bruker Nonius KappaCCD area-detector diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan (SORTAV; Blessing, 1997)  
*T<sub>min</sub>* = 0.802, *T<sub>max</sub>* = 0.837

9216 measured reflections  
 4974 independent reflections  
 3581 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.037  
 $\theta_{\text{max}}$  = 27.5°

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.036  
*wR*(*F*<sup>2</sup>) = 0.084  
*S* = 0.97  
 4974 reflections  
 237 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0404P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.61 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.79 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Sn1—O1 <sup>i</sup>	2.030 (3)	Sn2—C5	2.095 (4)
Sn1—C1	2.104 (4)	Sn2—C7	2.101 (4)
Sn1—C3	2.113 (4)	Sn2—O3	2.218 (3)
Sn1—O1	2.128 (3)	Sn2—O4	2.238 (3)
Sn1—O2 <sup>i</sup>	2.280 (3)	O2—C9	1.245 (5)
Sn1—O4	2.654 (3)	O3—C9	1.239 (5)
Sn2—O1	2.054 (3)		
O1 <sup>i</sup> —Sn1—C1	106.63 (15)	O1—Sn1—O4	67.29 (9)
O1 <sup>i</sup> —Sn1—C3	106.36 (14)	O2 <sup>i</sup> —Sn1—O4	126.25 (10)
C1—Sn1—C3	145.21 (19)	O1—Sn2—C5	104.20 (14)
O1 <sup>i</sup> —Sn1—O1	76.74 (11)	O1—Sn2—C7	102.44 (14)
C1—Sn1—O1	98.32 (15)	C5—Sn2—C7	153.34 (17)
C3—Sn1—O1	99.69 (14)	O1—Sn2—O3	91.70 (11)
O1 <sup>i</sup> —Sn1—O2 <sup>i</sup>	89.75 (11)	C5—Sn2—O3	88.71 (16)
C1—Sn1—O2 <sup>i</sup>	84.06 (17)	C7—Sn2—O3	89.67 (17)
C3—Sn1—O2 <sup>i</sup>	85.31 (15)	O1—Sn2—O4	77.33 (10)
O1—Sn1—O2 <sup>i</sup>	166.42 (11)	C5—Sn2—O4	92.66 (15)
O1 <sup>i</sup> —Sn1—O4	143.97 (10)	C7—Sn2—O4	93.96 (15)
C1—Sn1—O4	81.41 (14)	O3—Sn2—O4	168.95 (12)
C3—Sn1—O4	78.49 (13)		

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

Two C atoms of a cyclopentenyl ring were disordered over sites C18/C18' and C22/C22', with site occupancy factors of 0.706 (11) and 0.294 (11), respectively, for the unprimed and primed components of these atoms. These pairs of atoms were assigned the same anisotropic displacement parameters. H atoms were included in the refinement in geometrically idealized positions, with C—H = 0.95–1.00 Å and *U<sub>iso</sub>* =

1.5 (methyl H) and 1.2 (other H) times  $U_{eq}$  of the atoms to which they were bonded. The final difference map was free of any chemically significant features.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALE-PAK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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