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Key indicators

Single-crystal X-ray study
T = 150 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
R factor = 0.031
wR factor = 0.062
Data-to-parameter ratio = 29.3

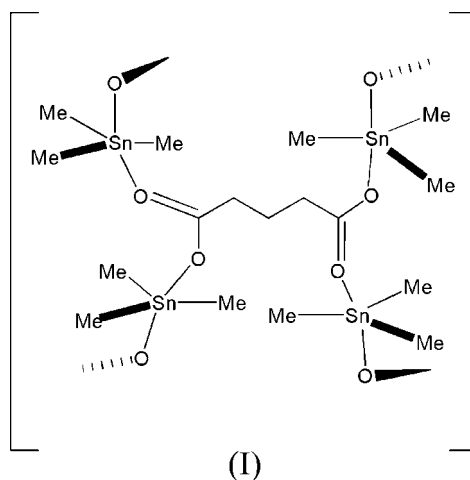
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Poly[bis(trimethyltin)- μ -glutarato]

The structure of $[\text{SnMe}_3\text{O}_2\text{C}(\text{CH}_2)_3\text{CO}_2\text{SnMe}_3]_n$ or $\{[\text{Sn}_2(\text{CH}_3)_6(\text{C}_5\text{H}_6\text{O}_4)]\}_n$ consists of an infinite layer containing pentacoordinate Sn atoms. There are two formula units, A and B, in the asymmetric unit. Glutarate acts as a tetradentate bridging ligand, each glutarate being linked to four different Sn atoms, generating two-dimensional sheets. One ligand links the Sn atoms of unit A, the other the Sn atoms of unit B. The sheets are parallel to each other.

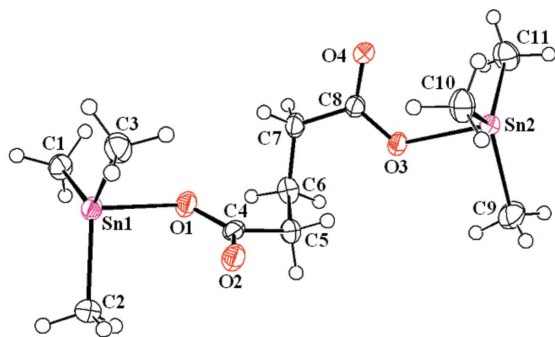
Comment

Crystal structures of $[\text{SnR}_3]_2[\text{O}_2\text{C}(\text{CH}_2)\text{CO}_2]$ ($R = \text{Me}$ and Ph) and $[\text{SnPh}_3]_2[\text{O}_2\text{C}(\text{CH}_2)_3\text{CO}_2]$ have been reported (Yin *et al.*, 2002; Cissé *et al.*, 2003). In addition to their interest as novel organotin species, bactericidal and fungicidal activity of triorganotin compounds are quite well known (Dutrecq *et al.*, 1992; Moens *et al.*, 1992). Such species are also screened for their antitumour activity and several of them are found to be active *in vitro* (Gielen, 2003, 2005). As a continuation of our interest in triaryltin derivatives (Diassé-Sarr *et al.*, 1997, 2004; Diop *et al.*, 2002), the X-ray crystallographic analysis of the title compound, (I) (Fig. 1), has been carried out and the results are presented here.

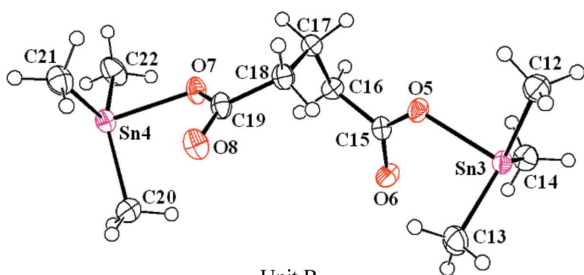


Each Sn atom is five-coordinate and adopts trigonal-bipyramidal $\text{trans-O}_2\text{SnC}_3$ geometry. There are two formula units in the asymmetric unit. The O—Sn—O bond angles are in the range $171.32(10)$ – $173.34(10)^\circ$ and are close to the ideal value, while C—Sn—C angles within the equatorial plane of the Sn atoms cover the range $117.35(17)$ – $123.25(18)^\circ$ and confirm the near-planarity of the SnC_3 groups revealed by the IR data. Each Sn atom has short [Sn1—O1 = $2.214(3) \text{ \AA}$] and long [Sn1—O2¹ = $2.346(3) \text{ \AA}$; symmetry code as in Table 1]

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Unit A



Unit B

Figure 1

The structures of the two formula units in the asymmetric unit of (I), with ellipsoids drawn at the 50% probability level. H atoms have been omitted.

Sn–O bond lengths, which correspond to two C–O bond lengths. The longer C–O bond [C4–O1 = 1.276 (5) Å] corresponds to the stronger Sn–O bond and the shorter C–O bond [C4–O2 = 1.244 (5) Å] to the longer (weaker) Sn–O bond (Table 1). In (I), the Sn–O bonds are slightly longer than those reported for the triphenyltin analogue (Yin *et al.*, 2002). The glutarate acts as a tetradentate bridging ligand, each glutarate being linked to four different Sn atoms, generating two-dimensional sheets. A first ligand links Sn1 and Sn2, another one Sn3 and Sn4. The sheets are parallel to each other (Fig. 2). The network incorporates 24-atom rectangular rings with approximate dimensions 9.9×6.7 Å measured between Sn atoms on opposite edges of the rectangle.

Experimental

Me₄NOH (10%), HCO₂(CH₂)₃CO₂H and SnMe₃Cl were obtained from Aldrich and were used without further purification. An ethanol solution (20 ml) containing [Me₄N]₂[CO₂(CH₂)₃CO₂]₂·5H₂O (0.37 g, 1 mmol) [obtained from a solution of Me₄NOH (20% in water) and HCO₂(CH₂)₃CO₂H in 1:2 ratio] and SnMe₃Cl (0.20 g, 1 mmol) was stirred at room temperature for more than 2 h to give a solution from which colourless crystals were formed after slow solvent evaporation (yield 80%; m.p. 391 K).

Crystal data

[Sn ₂ (CH ₃) ₆ (C ₅ H ₆ O ₄)]	$V = 3404.83$ (9) Å ³
$M_r = 457.68$	$Z = 8$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 10.0053$ (1) Å	$\mu = 2.94$ mm ⁻¹
$b = 13.1391$ (2) Å	$T = 150$ (2) K
$c = 25.9006$ (5) Å	$0.25 \times 0.25 \times 0.15$ mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan
(SORTAV; Blessing, 1995)
 $T_{\min} = 0.502$, $T_{\max} = 0.641$
42835 measured reflections
9389 independent reflections
8432 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.062$
 $S = 1.04$
9389 reflections
320 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.72$ e Å⁻³
 $\Delta\rho_{\min} = -1.11$ e Å⁻³
Absolute structure: Flack (1983),
3866 Friedel pairs
Flack parameter: 0.50 (2)

Table 1

Selected geometric parameters (Å, °).

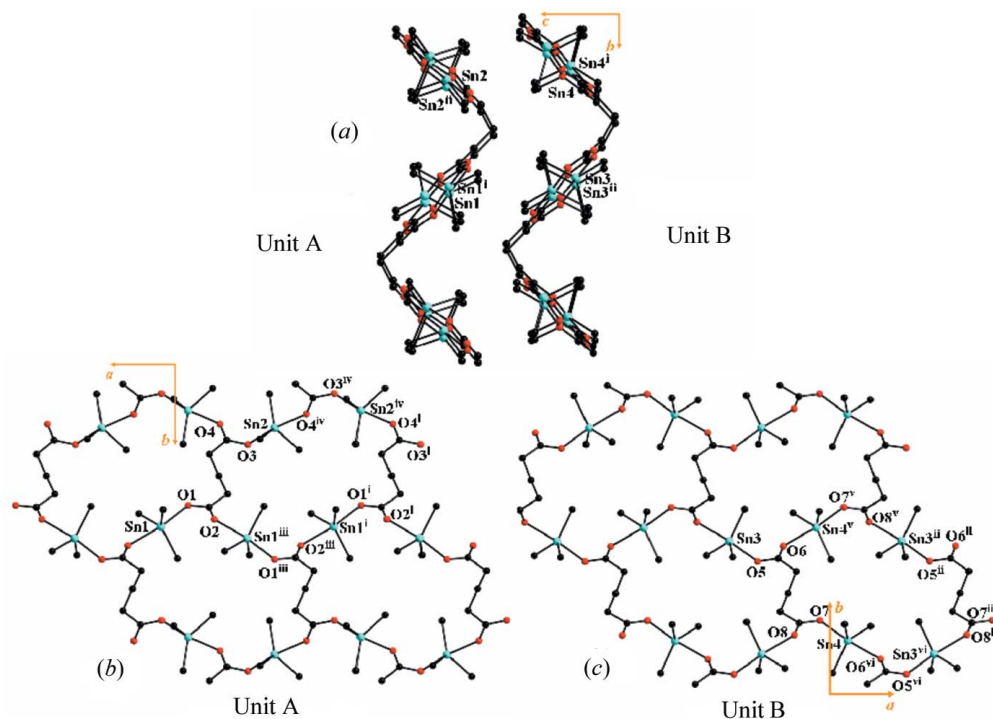
Sn1–O1	2.214 (3)	O2–C4	1.244 (5)
Sn1–O2 ⁱ	2.346 (3)	O3–C8	1.270 (5)
Sn2–O3	2.201 (3)	O4–C8	1.258 (5)
Sn2–O4 ⁱⁱ	2.333 (3)	O5–C15	1.276 (5)
Sn3–O5	2.197 (3)	O6–C15	1.243 (5)
Sn3–O8 ⁱⁱⁱ	2.343 (3)	O7–C19	1.268 (5)
Sn4–O7	2.211 (3)	O8–C19	1.255 (5)
O1–C4	1.276 (5)		
C1–Sn1–C2	117.35 (17)	C10–Sn2–O3	94.60 (14)
C1–Sn1–C3	119.91 (18)	C10–Sn2–O4 ⁱⁱ	88.79 (14)
C3–Sn1–C2	122.34 (18)	C11–Sn2–O3	95.74 (15)
C10–Sn2–C9	118.3 (2)	C11–Sn2–O4 ⁱⁱ	88.60 (14)
C11–Sn2–C10	122.02 (19)	C12–Sn3–O5	88.33 (14)
C11–Sn2–C9	119.1 (2)	C12–Sn3–O8 ⁱⁱⁱ	85.05 (14)
C13–Sn3–C12	119.36 (19)	C13–Sn3–O5	94.11 (14)
C14–Sn3–C13	123.19 (18)	C13–Sn3–O8 ⁱⁱⁱ	88.54 (14)
C14–Sn3–C12	117.01 (19)	C14–Sn3–O5	93.89 (14)
C20–Sn4–C21	123.25 (18)	C14–Sn3–O8 ⁱⁱⁱ	89.75 (14)
C22–Sn4–C20	118.79 (19)	C20–Sn4–O6 ^{iv}	87.64 (14)
C22–Sn4–C21	117.4 (2)	C21–Sn4–O6 ^{iv}	89.90 (14)
C1–Sn1–O1	86.64 (13)	C20–Sn4–O7	95.28 (14)
C1–Sn1–O2 ⁱ	85.01 (13)	C21–Sn4–O7	94.41 (14)
C2–Sn1–O1	95.15 (14)	C22–Sn4–O6 ^{iv}	84.66 (14)
C2–Sn1–O2 ⁱ	90.80 (14)	C22–Sn4–O7	87.70 (14)
C3–Sn1–O1	94.33 (14)	O1–Sn1–O2 ⁱ	171.32 (10)
C3–Sn1–O2 ⁱ	87.79 (15)	O3–Sn2–O4 ⁱⁱ	171.96 (10)
C9–Sn2–O3	87.29 (15)	O5–Sn3–O8 ⁱⁱⁱ	173.34 (10)
C9–Sn2–O4 ⁱⁱ	84.68 (15)	O7–Sn4–O6 ^{iv}	172.31 (10)

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 2$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 2$; (iii) $-x - 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.

The structure was refined as an inversion twin, with components in the ratio 1:1. All H atoms were geometrically located in ideal positions and refined using a riding model, with C–H = 0.98 Å for methyl H atoms and C–H = 0.99 Å for methylene H atoms, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene H atoms. The deepest hole in the final difference map is 0.78 Å from Sn4.

Data collection: COLLECT (Nonius, 1997); cell refinement: HKL SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1998); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Figure 2

(a) A view along the *a* axis of the structure of (I), showing the two units. (b) A view along the *b* axis of unit A, showing the two-dimensional sheet incorporating Sn1 and Sn2. (c) A view along the *b* axis of unit B, showing the two-dimensional sheet incorporating Sn3 and Sn4. [Symmetry codes: (i) $x - 1, y, z$; (ii) $x + 1, y, z$; (iii) $x - \frac{1}{2}, \frac{3}{2} - y, 2 - z$; (iv) $x - \frac{1}{2}, \frac{1}{2} - y, 2 - z$; (v) $-x, 1/2 + y, \frac{3}{2} - z$; (vi) $-x, y - \frac{1}{2}, \frac{3}{2} - z$.]

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