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Polymeric di-*n*-butyl(glutarato)tin(IV)

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The crystal structure of *catena*-poly[[di-*n*-butyltin(IV)]-μ-glutarato], [Sn(C_4H_9)$_2$($C_5H_6O_4$)], is composed of polymeric chains formed by coordination of glutarate, through both ends, to di-*n*-butyltin. The geometry around the hexacoordinated Sn atom is highly distorted octahedral, and may best be described as based on a skew-trapezoidal planar geometry. The symmetry-related glutarate ligands are asymmetrically coordinated to the Sn atoms, with Sn—O distances of 2.138 (2) and 2.483 (2) Å. The Sn—C distance involving the *n*-butyl group is 2.124 (3) Å.

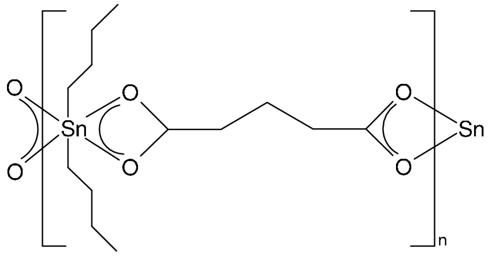
Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.005 Å
R factor = 0.028
wR factor = 0.066
Data-to-parameter ratio = 14.6

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

Comment

Since the discovery of the anticancer activity of platinum complexes (Rosenberg *et al.*, 1969), there has been an extensive effort to identify organic complexes of other metals possessing anticancer activity (Cleare, 1974). There have been several reports of anticancer activity for certain organotin complexes (Crowe *et al.*, 1984; Cardin & Roy, 1985; Huber *et al.*, 1985). Organotin compounds have displayed other biological activities, *e.g.* they are widely used as fungicides, pesticides, antifouling coatings, polymer stabilizers and wood preservatives (Jousseaume *et al.*, 1993; Davies & Smith, 1982; Parulekar *et al.*, 1990; Molloy *et al.*, 1986, 1987; Kumari *et al.*, 1994). Organotin compounds have also shown antibacterial and antifungal properties and are powerful biocides (Danish *et al.*, 1995). We have been interested in the synthesis, characterization, biological applications and crystal structures of organotin carboxylates. Therefore, we have prepared *catena*-poly[[di-*n*-butyltin(IV)]-μ-glutarato], (I), and report its structure here.



(I)

The structure of (I) is composed of polymeric chains formed by the coordination of glutarate anions, through both ends, to di-*n*-butyltin (Fig. 1). The Sn atom lies on a special position so that only half of the molecule constitutes the asymmetric unit. The hexacoordinated Sn atom is surrounded by four glutarate O atoms, forming an almost square base, with the *n*-butyl ligands occupying the two axial positions. The geometry around the Sn atom is highly distorted octahedral, and may

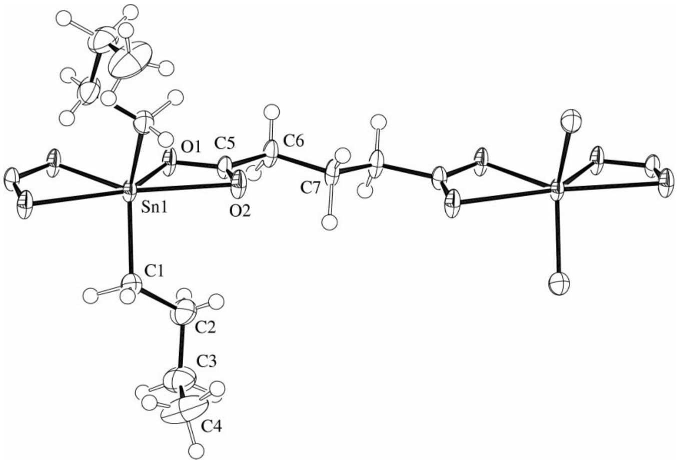


Figure 1
*ORTEP*II (Johnson, 1976) drawing of the polymeric chain of (I), with displacement ellipsoids plotted at the 50% probability level.

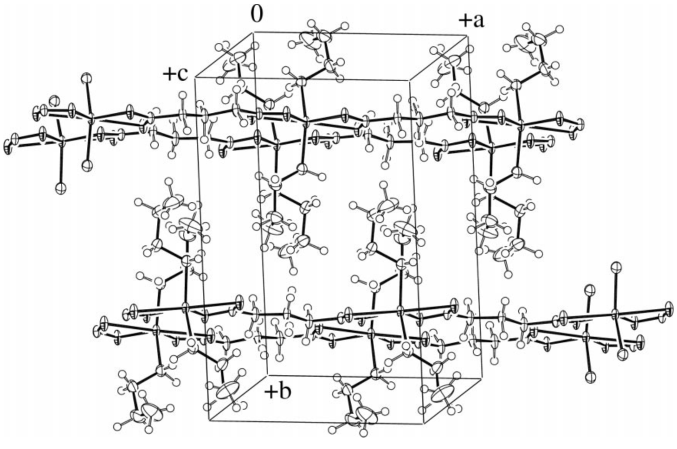


Figure 2
The unit-cell packing for (I).

best be described as based on a skew-trapezoidal planar geometry (Table 1). The symmetry-related glutarate ligands are asymmetrically coordinated to the Sn atoms, with Sn—O distances of 2.138 (2) and 2.483 (2) Å. The Sn—C distance involving the *n*-butyl group is 2.124 (3) Å. The C—O distances are significantly different, 1.295 (3) and 1.234 (3) Å, and correspond to strongly and weakly coordinated O atoms, respectively. A similar pattern of Sn—O and C—O bond distances has been reported for the crystal structures of diorganotin(IV) carboxylates (Lockhart *et al.*, 1987), $[Sn(C_2H_5)_2(C_7H_5O_2S)_2]$ (Parvez *et al.*, 1997) and $[Me_2Sn(O_2CPh)_2]$ (Tiekink, 1991).

The structure of (I) is devoid of any hydrogen bonds and the molecules are packed in the unit cell, forming chains of Sn–glutarate along the *a* axis; the *n*-butyl groups attached to Sn atoms fill the gaps between these chains (Fig. 2).

Experimental

Glutaric anhydride (1.14 g, 1 mmol) was dissolved in toluene (50 ml) and ethanol (15 ml), and di-*n*-butyltin oxide (1.24 g, 5 mmol) was added. The mixture was refluxed for 6 h and the ternary azeotrope water/ethanol/toluene was distilled off using a Dean–Stark funnel. Half of the remaining solution was evaporated under vacuum. The oily compound thus obtained was allowed to crystallize from chloroform–methanol (1:1) at room temperature by slow evaporation, yielding crystals of (I) suitable for X-ray diffraction studies.

Crystal data

$[Sn(C_4H_9)_2(C_5H_6O_4)]$
$M_r = 363.02$
Orthorhombic, *Pccn*
$a = 9.9698\ (4)$ Å
$b = 15.6977\ (4)$ Å
$c = 9.9088\ (8)$ Å
$V = 1550.76\ (15)$ Å^3
$Z = 4$
$D_x = 1.555$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5771 reflections
$\theta = 1.0$–27.5°
$\mu = 1.65$ mm^{-1}
$T = 223\ (2)$ K
Plate, colourless
0.27 × 0.24 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{\min} = 0.664$, $T_{\max} = 0.866$
5771 measured reflections
1727 independent reflections
1462 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$
$\theta_{\max} = 27.5°$
$h = -12 \rightarrow 11$
$k = -20 \rightarrow 20$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.066$
$S = 1.19$
1727 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 3.123P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.54$ e Å^{-3}
$\Delta\rho_{\min} = -0.51$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0189 (17)

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.124 (3)	O1—C5	1.295 (3)
Sn1—O1	2.138 (2)	O2—C5	1.234 (3)
Sn1—O2	2.483 (2)		
C1—Sn1—C1$^{\rm i}$	138.84 (17)	C1—Sn1—O2	91.81 (10)
C1—Sn1—O1	104.98 (10)	O1—Sn1—O2	55.83 (7)
C1$^{\rm i}$—Sn1—O1	106.68 (10)	O2$^{\rm i}$—Sn1—O2	170.49 (9)
O1—Sn1—O1$^{\rm i}$	78.20 (10)	C5—O1—Sn1	99.52 (15)
C1—Sn1—O2$^{\rm i}$	84.85 (10)	C5—O2—Sn1	85.11 (16)
O1—Sn1—O2$^{\rm i}$	133.66 (7)		

Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, z$.

The H atoms were located from difference Fourier syntheses and were included in the refinements with an overall isotropic displacement parameter, with the exception of the H atoms attached to C7, which were included at geometrically idealized positions.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *HKL DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI*91 (Fan, 1991); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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