

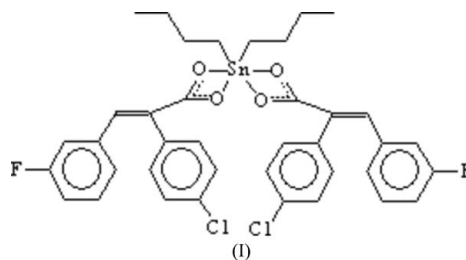
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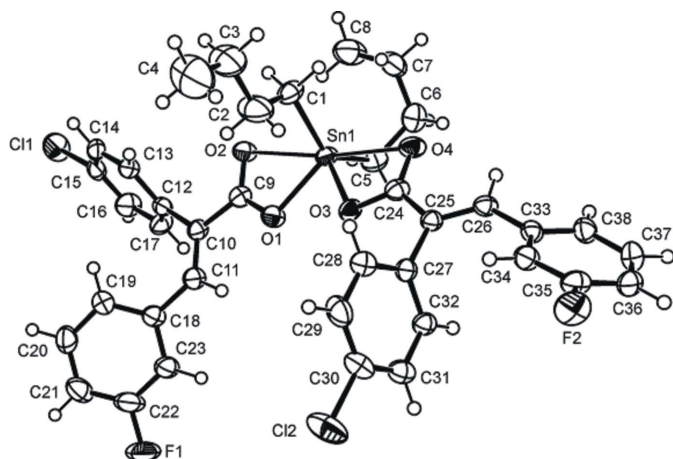
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## Key indicators

Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
Disorder in main residue  
 $R$  factor = 0.039  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 18.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Di-*n*-butylbis[(*E*)-2-(4-chlorophenyl)-3-(3-fluoro-  
phenyl)prop-2-enoato- $\kappa^2\text{O},\text{O}$ ]tin(IV)The molecule of the title compound,  $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_{15}\text{H}_9\text{ClFO}_2)_2]$ , has a skewed-trapezoidal planar geometry, defined by four O donors from the carboxylate ligands and two C atoms from the *n*-butyl groups. The C—Sn—C bond angle is  $133.95(12)^\circ$ . The O atoms of the carboxylate ligands are bonded asymmetrically to Sn, with significantly different Sn—O distances; the values for the shorter are 2.0914 (18) and 2.1134 (19) Å, while the longer Sn—O distances are 2.513 (2) and 2.650 (2) Å.Received 23 March 2006  
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## Comment

The study of organotin compounds with biologically important ligands has gained importance due to the potential pharmaceutical applications of organotin compounds (Anderson *et al.*, 1984). The biological applications of organotin compounds as antitumour and anticancer agents (Yang & Guo, 1999; Gielen *et al.*, 2002) and the structural aspects of organotin carboxylates have been well documented (Tiekink, 1994; Hans *et al.*, 2002). We report here the crystal structure of the title compound, (I), as a continuation of our efforts in the synthesis and structural characterization of organotin carboxylates (Sadiq-ur-Rehman *et al.*, 2004).The structure of (I) is composed of discrete monomeric molecules, in which four O atoms of the carboxylate ligands and two C atoms of the *n*-butyl groups surround the hexacoordinated Sn atom (Fig. 1). The Sn atom lies in the same plane as the four O atoms coordinated to it, and the two *n*-butyl groups lie above and below this plane. The C1—Sn1—C5 angle in (I) is  $133.95(12)^\circ$ , which is comparable with the corresponding angle in similar structures (Gibson *et al.*, 1997). The Sn—C distances are identical within the  $3\sigma$  limit [mean Sn—C 2.107 (3) Å]. On the other hand, the propenoate ligands are asymmetrically coordinated to Sn, with Sn—O distances significantly different from each other (Table 1).The geometry around the Sn atom is highly distorted octahedral, which may be best described as based on a skewed-trapezoidal planar geometry. The bond distances and angles involving the Sn atom in (I) are in agreement with the corresponding values found for a similar Sn complex (Hans *et*



**Figure 1**  
The structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

*al.*, 2002) in the Cambridge Structural Database (CSD, Version 5.26; Allen, 2002). The molecular dimensions in the *E*-3-(3-fluorophenyl)-2-(4-chlorophenyl)-2-propenoate ligand are normal, with mean distances of C=C 1.338 (4) Å and  $C_{sp^2}-C_{sp^2}$  1.492 (4) Å. The C—O bond distances in the delocalized region of the carboxylate groups are significantly different from each other. These distances for the weakly coordinated O atoms are shorter [mean 1.244 (3) Å] than the C—O distances of the strongly bound O atoms [mean 1.299 (3) Å].

## Experimental

Di-*n*-butyltin oxide (1.0 g, 4 mmol) and the ligand *E*-3-(3-fluorophenyl)-2-(4-chlorophenyl)-2-propenoic acid (2.21 g, 8 mmol) were suspended in dry toluene (100 ml) in a single-necked round-bottomed flask (250 ml) equipped with a Dean–Stark funnel, magnetic stirrer and water condenser. The mixture was refluxed for 8–10 h and water formed during the condensation reaction was removed at intervals *via* the Dean–Stark separator. The mixture was then cooled to room temperature and the solvent was removed using a rotary evaporator. The solid collected was recrystallized from a solution in a mixture of chloroform and *n*-hexane (4:1) by slow evaporation at room temperature.

### Crystal data

$[Sn(C_4H_9)_2(C_{15}H_9ClFO_2)_2]$	$D_x = 1.459 \text{ Mg m}^{-3}$
$M_r = 784.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 15031 reflections
$a = 11.252 (2) \text{ \AA}$	$\theta = 3.5\text{--}27.5^\circ$
$b = 11.886 (2) \text{ \AA}$	$\mu = 0.92 \text{ mm}^{-1}$
$c = 26.932 (4) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\beta = 97.470 (8)^\circ$	Block, colourless
$V = 3571.4 (10) \text{ \AA}^3$	$0.24 \times 0.18 \times 0.16 \text{ mm}$
$Z = 4$	

### Data collection

Nonius KappaCCD area-detector diffractometer	8137 independent reflections
$\omega$ and $\varphi$ scans	5376 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SORTAV; Blessing, 1997)	$R_{int} = 0.047$
$T_{min} = 0.811$ , $T_{max} = 0.868$	$\theta_{max} = 27.5^\circ$
15031 measured reflections	$h = -14 \rightarrow 14$
	$k = -15 \rightarrow 15$
	$l = -34 \rightarrow 34$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2]$
$wR(F^2) = 0.085$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
8137 reflections	$\Delta\rho_{max} = 0.74 \text{ e \AA}^{-3}$
434 parameters	$\Delta\rho_{min} = -0.79 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Sn1—O1	2.0914 (18)	Cl1—C15	1.742 (3)
Sn1—C1	2.104 (3)	Cl2—C30	1.751 (3)
Sn1—C5	2.110 (3)	O1—C9	1.299 (3)
Sn1—O3	2.1134 (19)	O2—C9	1.241 (3)
Sn1—O4	2.513 (2)	O3—C24	1.298 (3)
Sn1—O2	2.650 (2)	O4—C24	1.247 (3)
O1—Sn1—C1	110.82 (11)	O1—Sn1—O2	53.99 (7)
O1—Sn1—C5	102.83 (10)	C1—Sn1—O2	84.92 (10)
C1—Sn1—C5	133.95 (12)	C5—Sn1—O2	90.56 (10)
O1—Sn1—O3	80.05 (7)	O3—Sn1—O2	132.60 (7)
C1—Sn1—O3	103.61 (10)	O4—Sn1—O2	171.52 (6)
C5—Sn1—O3	112.59 (11)	C9—O1—Sn1	104.89 (16)
O1—Sn1—O4	134.35 (7)	C9—O2—Sn1	80.33 (17)
C1—Sn1—O4	92.06 (10)	C24—O3—Sn1	101.06 (16)
C5—Sn1—O4	85.84 (10)	C24—O4—Sn1	83.88 (17)
O3—Sn1—O4	55.82 (7)		

H atoms were positioned geometrically, with C—H distances in the range 0.95–0.99 Å, and treated as riding, with  $U_{iso}(H) = 1.2U_{eq}(C)$ , or  $1.5U_{eq}(C)$  for methyl H.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (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*.

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