

## (4-Chloro-3,5-dinitrobenzoato)triphenyltin(IV)

Aziz-ur-Rehman,<sup>a</sup> Madeleine Helliwell,<sup>b</sup> Saqib Ali<sup>a\*</sup> and Saira Shahzadi<sup>a</sup><sup>a</sup>Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and<sup>b</sup>School of Chemistry, The University of Manchester, Manchester M13 9PL, England

Correspondence e-mail: drsa54@yahoo.com

## Key indicators

Single-crystal X-ray study

T = 100 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.026

wR factor = 0.068

Data-to-parameter ratio = 15.1

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

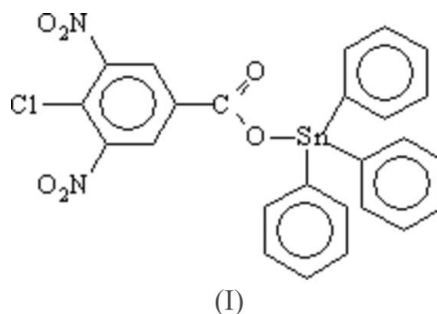
The geometry around the Sn atom of the title compound,  $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_7\text{H}_2\text{ClN}_2\text{O}_6)]$ , is distorted tetrahedral, with Sn—C distances lying in the range 2.124 (2)–2.119 (2) Å and an Sn—O distance of 2.0645 (15) Å.

Received 9 June 2006

Accepted 20 June 2006

## Comment

Organotin compounds are of current interest due to their dramatic increase of industrial, agricultural and biological applications (Xie *et al.*, 1996; Nath *et al.*, 2001). Studies of organotin and biologically important ligands have gained importance due to potential pharmaceutical applications of organotin compounds (Anderson *et al.*, 1984). The biological applications of organotin compounds as antitumor 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(IV) carboxylates (Sadiq-ur-Rehman *et al.*, 2006).

The structure of (I) is composed of discrete monomeric molecules in which the O atom of the carboxylate ligand and three C atoms of three phenyl groups surround the tetra-coordinated Sn atom (Fig. 1). The Sn atom exists in a distorted tetrahedral geometry. The largest distortion from the ideal tetrahedral geometry is found in the O1—Sn—C8 angle (Table 1); the C14—Sn1—C20 angle shows the next largest distortion from the ideal geometry. The monodentate mode of coordination of the 4-chloro-3,5-dinitrobenzoate is reflected in the disparate O1—C1 and O2—C2 bond distances, with the longer bond associated with the stronger Sn1—O1 interaction. The bond distances and angles involving the Sn atom are in agreement with the corresponding values found for similar Sn complexes (Sadiq-ur-Rehman *et al.*, 2005).

## Experimental

Triphenyltin(IV) hydroxide (0.6 g, 2.4 mmol) and 3,5-dinitro-4-chlorobenzoic acid (0.9 g, 2.4 mmol) were suspended in dry toluene (150 ml) in a two-necked round-bottomed flask equipped with a water condenser. The mixture was refluxed for 8–10 h and the water that formed during the condensation reaction was periodically removed *via* a Dean–Stark separator. The mixture was cooled to room temperature and solvent was removed on a rotary evaporator under reduced pressure. The solid product was recrystallized from chloroform to obtain colourless crystals suitable for X-ray analysis (yield 75%; m.p. 414–416 K).

### Crystal data

[Sn(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> (C <sub>7</sub> H <sub>2</sub> ClN <sub>2</sub> O <sub>6</sub> )]	Z = 4
<i>M<sub>r</sub></i> = 595.55	<i>D<sub>x</sub></i> = 1.698 Mg m <sup>-3</sup>
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Mo K $\alpha$ radiation
<i>a</i> = 12.7457 (8) Å	$\mu$ = 1.26 mm <sup>-1</sup>
<i>b</i> = 8.3919 (5) Å	<i>T</i> = 100 (2) K
<i>c</i> = 22.3719 (14) Å	Block, colourless
$\beta$ = 103.1560 (10)°	0.40 × 0.35 × 0.35 mm
<i>V</i> = 2330.1 (2) Å <sup>3</sup>	

### Data collection

Bruker SMART CCD area-detector diffractometer	13029 measured reflections
$\varphi$ and $\omega$ scans	4757 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	4272 reflections with <i>I</i> > 2 $\sigma$ ( <i>I</i> )
<i>T</i> <sub>min</sub> = 0.633, <i>T</i> <sub>max</sub> = 0.668	<i>R</i> <sub>int</sub> = 0.029
	$\theta$ <sub>max</sub> = 26.4°

### Refinement

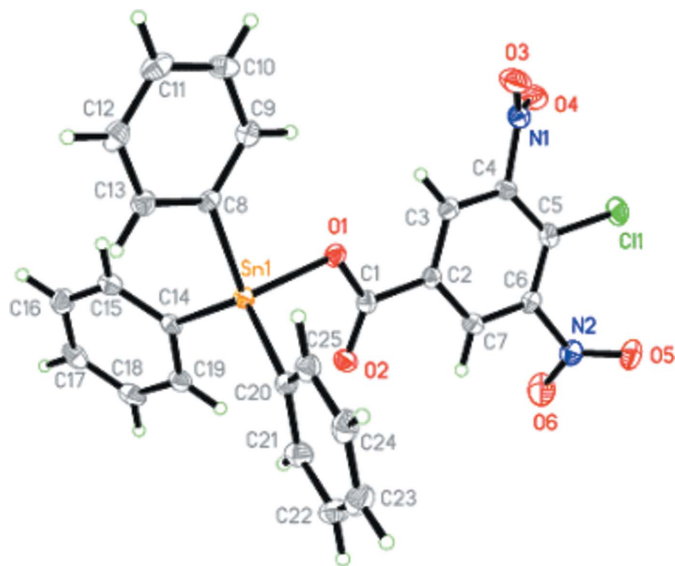
Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.1522P]$
$R[F^2 > 2\sigma(F^2)] = 0.026$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.068$	( $\Delta/\sigma$ ) <sub>max</sub> = 0.001
<i>S</i> = 1.03	$\Delta\rho$ <sub>max</sub> = 1.25 e Å <sup>-3</sup>
4757 reflections	$\Delta\rho$ <sub>min</sub> = -0.35 e Å <sup>-3</sup>
316 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

Sn1—O1	2.0654 (15)	Sn1—C8	2.124 (2)
Sn1—C14	2.119 (2)	O1—C1	1.305 (3)
Sn1—C20	2.120 (2)	O2—C1	1.221 (3)
O1—Sn1—C14	110.48 (7)	O1—Sn1—C8	97.64 (7)
O1—Sn1—C20	103.46 (7)	C14—Sn1—C8	111.21 (8)
C14—Sn1—C20	119.25 (9)	C20—Sn1—C8	112.28 (9)

H atoms were included in calculated positions and refined as riding, with C—H distances of 0.95 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The highest density peak is located 0.11 Å from atom H10.



**Figure 1**

The structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

AR is thankful to HEC (Higher Education Commission, Islamabad, Pakistan) for financial support under PhD Fellowship Scheme Batch-II (PIN Code: 042-111621-PS2-179).

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