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## Key indicators

Single-crystal X-ray study  
 $T = 295\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
Disorder in main residue  
 $R$  factor = 0.051  
 $wR$  factor = 0.110  
Data-to-parameter ratio = 15.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

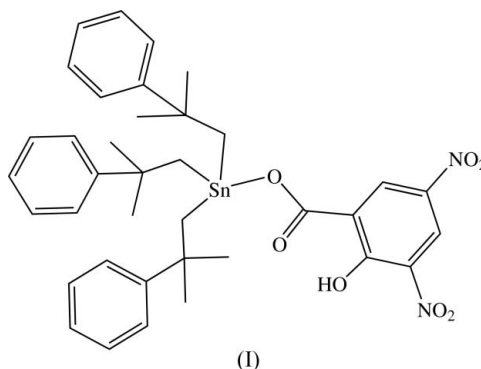
## (2-Hydroxy-3,5-dinitrobenzoato)tris(2-methyl-2-phenylpropyl)tin(IV)

The Sn atom of the title compound,  $[\text{Sn}(\text{C}_{10}\text{H}_{13})_3(\text{C}_7\text{H}_3\text{N}_2\text{O}_7)]$ , is four-coordinate and possesses a distorted tetrahedral geometry. There is an intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond between the carboxyl and the phenolic hydroxy groups.

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## Comment

Recently, we have reported several structures of tris(2-methyl-2-phenylpropyl)tin carboxylates, such as tris(2-methyl-2-phenylpropyl)tin pyridine-3-carboxylate (Tian, Sun, Yang & Yang, 2005), 3,5-dinitrobenzoate (Tian, Yu, Sun, & Zhang, 2005) and bis[tris(2-methyl-2-phenylpropyl)tin(IV)] phthalate (Tian, Sun, Yang & Ng, 2005), which all possess a distorted tetrahedral geometry. In the title compound, (I), tetrahedral coordination is also observed (Fig. 1).



The  $\text{Sn1}\cdots\text{O2}$  separation of  $3.118(3)\text{ \AA}$  indicates a weak interaction between these atoms, which distorts the tetrahedral geometry. Bond dimensions around the Sn atom (Table 1) are similar to those found in the carboxylate structures mentioned above. An intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond is observed between the carboxyl and the phenolic hydroxy groups (Fig. 1 and Table 2). The OH group is disordered over two *ortho* positions, and both O atoms of the carboxylate functionality may serve as acceptor for the intramolecular hydrogen bonding, giving hydrogen bonds of very similar strengths. An unbalanced statistical distribution,  $0.836(7)/0.164(7)$ , clearly reflects the fact that atom O2 is a better acceptor than O1.

## Experimental

Bis[tris(2-methyl-2-phenylpropyl)tin] oxide (1.05 g, 1 mmol) and 2-hydroxy-3,5-dinitrobenzoic acid (0.46 g, 2 mmol) in toluene (50 ml) were refluxed for 5 h with azeotropic removal of water *via* a Dean-Stark trap. The resulting clear solution was evaporated under reduced pressure. The white solid obtained, (I), was purified by recrystal-

lization from ethanol and crystals were obtained from a chloroform-hexane (1:1 *v/v*) solution by slow evaporation at 298 K (yield 73%, m.p. 382–383 K). Analysis found: C 59.76, H 5.59, N 3.65%; calculated for C<sub>37</sub>H<sub>42</sub>N<sub>2</sub>O<sub>7</sub>Sn: C 59.61, H 5.68, N 3.76%. IR (KBr disc):  $\nu_{\text{as}}(\text{CO}_2)$  1651,  $\nu_{\text{s}}(\text{CO}_2)$  1340,  $\nu_{\text{as}}(\text{NO}_2)$  1536,  $\nu_{\text{s}}(\text{NO}_2)$  1398 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS as reference):  $\delta$  9.31 (2H, *s*, nitrobenzene H), 7.28–7.05 (15H, *m*, 3 × C<sub>6</sub>H<sub>5</sub>), 5.17 (1H, *s*, OH), 1.30 (6H, *s*, 3 × CH<sub>2</sub>Sn), 1.24 (18H, *s*, 6 × CH<sub>3</sub>); <sup>119</sup>Sn NMR (111.9 MHz, CDCl<sub>3</sub>, Me<sub>4</sub>Sn as reference):  $\delta$  112.3.

Crystal data

[Sn(C<sub>10</sub>H<sub>13</sub>)<sub>3</sub>(C<sub>7</sub>H<sub>3</sub>N<sub>2</sub>O<sub>7</sub>)]  
*M<sub>r</sub>* = 745.42  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 10.0060 (8) Å  
*b* = 22.6236 (18) Å  
*c* = 15.8991 (13) Å  
 $\beta$  = 95.512 (1)°  
*V* = 3582.5 (5) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.382 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 7082 reflections  
 $\theta$  = 2.3–25.6°  
 $\mu$  = 0.76 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Needle, pale yellow  
 0.25 × 0.10 × 0.08 mm

Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
*T<sub>min</sub>* = 0.832, *T<sub>max</sub>* = 0.942  
 26672 measured reflections

6649 independent reflections  
 5673 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.040  
 $\theta_{\text{max}}$  = 25.5°  
*h* = -12 → 12  
*k* = -27 → 26  
*l* = -19 → 19

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.051  
*wR* (*F*<sup>2</sup>) = 0.110  
*S* = 1.18  
 6649 reflections  
 434 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.8962P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.91 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.79 \text{ e \AA}^{-3}$

Table 1 Selected geometric parameters (Å, °).

Sn1—O1	2.109 (3)	O2—C1	1.242 (5)
Sn1—C18	2.144 (4)	O7A—C3	1.326 (5)
Sn1—C8	2.146 (4)	O7B—C7	1.393 (17)
Sn1—C28	2.147 (4)	C1—C2	1.479 (5)
O1—C1	1.273 (5)		
O1—Sn1—C18	104.07 (14)	O1—Sn1—C28	90.41 (15)
O1—Sn1—C8	101.84 (15)	C18—Sn1—C28	118.70 (17)
C18—Sn1—C8	116.22 (16)	C8—Sn1—C28	118.25 (17)

Table 2 Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O7B—H7BA...O1	0.82	1.74	2.465 (18)	147
O7A—H7AA...O2	0.82	1.73	2.477 (4)	150

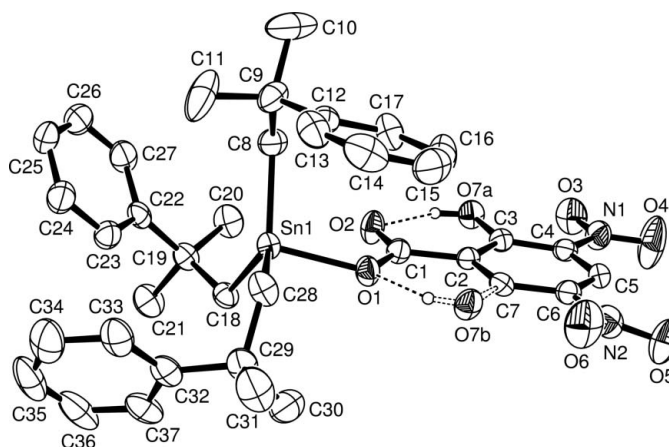


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The disordered hydroxy group (O7a/O7b) is represented with different bond styles. Except for the OH groups, H atoms have been omitted. Hydrogen bonds are shown as dashed lines.

The hydroxyl group of the hydroxydinitrobenzoate ligand is disordered over two sites. Site-occupation factors were refined with a sum constrained to 1, converging to 0.836 (7) for atom O7a and 0.164 (7) for O7b. H atoms were placed at calculated positions and were included in the refinement in the riding-model approximation [C—H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for aromatic H atoms; C—H = 0.96 Å and *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C) for methyl H atoms; C—H = 0.97 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for methylene H atoms; O—H = 0.82 Å and *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(O) for hydroxy H atoms].

Data collection: SMART (Bruker, 2002); 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: ORTEP3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97 (Bruker, 2002).

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