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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.015 \text{ \AA}$   
 R factor = 0.041  
 wR factor = 0.111  
 Data-to-parameter ratio = 11.8

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

**Rerefinement of *catena*-poly[triethylammonium  
 [triphenylstannate(IV)- $\mu$ -2,5-thiophenedicarboxylato]]  
 in the space group *Pc***

The structure of the title compound,  $\{(\text{C}_6\text{H}_{15}\text{N})[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_6\text{H}_2\text{O}_4\text{S})]\}_n$ , when refined in *Pc*, comprises two independent formula units. The polyanionic chain has both Sn atoms in *trans*- $\text{C}_3\text{SnO}_2$  trigonal-bipyramidal geometries.

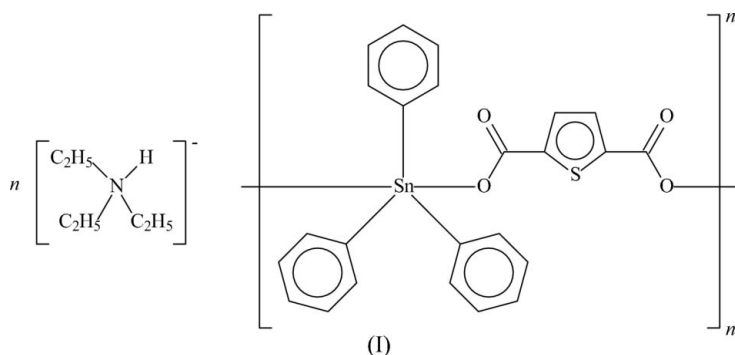
Received 26 October 2005

Accepted 31 October 2005

Online 5 November 2005

**Comment**

The structure of  $[(\text{C}_2\text{H}_5)_3\text{NH}][(\text{C}_6\text{H}_5)_3\text{Sn}(\text{C}_6\text{H}_2\text{O}_4\text{S})]$ , (I), a compound belonging to the class of polymeric (dicarboxylato)triorganostannates which is expected to exhibit aqueous solubility (Ng & Kumar Das, 1997), was originally refined in space group *P1* with four independent formula units to *R* 0.040 (Ma *et al.*, 2004). The triclinic cell can be transformed to a monoclinic cell. In the monoclinic *Pc* setting, the two independent triphenyltin units are linked by the two 2,5-thiophenedicarboxylates into a linear chain (Fig. 1 and Table 1). The cations are hydrogen-bonded to the chains, as detailed in Table 2. The polyanionic chain has both Sn atoms in *trans*- $\text{C}_3\text{SnO}_2$  trigonal bipyramidal geometries.



**Experimental**

*Crystal data*

$(\text{C}_6\text{H}_{15}\text{N})[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_6\text{H}_2\text{O}_4\text{S})]$   
 $M_r = 622.32$   
 Monoclinic, *Pc*  
 $a = 18.354 (4) \text{ \AA}$   
 $b = 9.658 (2) \text{ \AA}$   
 $c = 18.982 (3) \text{ \AA}$   
 $\beta = 119.69 (2)^\circ$   
 $V = 2923 (1) \text{ \AA}^3$   
 $Z = 4$

$D_x = 1.414 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 846  
 reflections  
 $\theta = 2.4\text{--}23.6^\circ$   
 $\mu = 0.98 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 Block, colorless  
 $0.25 \times 0.14 \times 0.07 \text{ mm}$

*Data collection*

Bruker SMART area-detector  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.792, T_{\max} = 0.935$   
 14964 measured reflections

7034 independent reflections  
 5750 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -21 \rightarrow 17$   
 $k = -11 \rightarrow 11$   
 $l = -21 \rightarrow 22$

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.041$  $wR(F^2) = 0.111$  $S = 1.03$ 

7034 reflections

595 parameters

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

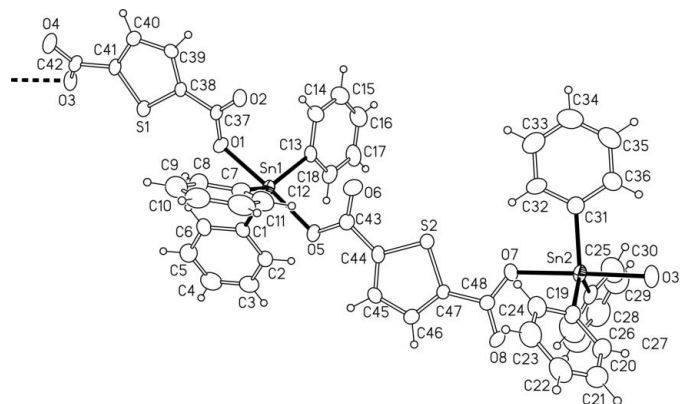
$$\Delta\rho_{\max} = 0.84 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack (1983),

from 1284 Friedel pairs

Flack parameter: 0.01 (3)



**Figure 1**  
ORTEP (Johnson, 1976) plot of the polyanionic  $[(C_6H_5)_3Sn(O_2CC_4H_2SCO_2)]_n$  chain. Displacement ellipsoids are drawn at the 30% probability level. The two cations are not shown. [Symmetry code (i) =  $x - 1, y - 1, z - 1$ .]

The H atoms were positioned geometrically (C–H 0.93 to 0.97, N–H 0.91 Å) and were included in the refinement in the riding-model approximation, with  $U(H)$  set to 1.2 to 1.5 times  $U_{eq}(C, N)$ .

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINTE* (Bruker, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

I thank Professor Chun-Lin Ma of Liaocheng Teachers University for the diffraction data, and the University of Malaya for supporting this study.

## References

- Bruker (1996). *SAINTE* and *SMART*. Bruker Analytical X-Ray Systems, Inc., Madison, Wisconsin, USA.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Johnson, C. K. (1976). *ORTEP*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
 Ma, C.-L., Sun, J.-F., Qui, L.-L. & Cui, J.-C. (2004). *J. Inorg. Organomet. Polym.* **14**, 161–168.  
 Ng, S. W. & Kumar Das, V. G. (1997). *Trends Organomet. Chem.* **2**, 107–115.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

**Table 1**

Selected geometric parameters (Å, °).

Sn1–C1	2.157 (4)	Sn2–C19	2.154 (4)
Sn1–C7	2.150 (4)	Sn2–C25	2.127 (6)
Sn1–C13	2.155 (4)	Sn2–C31	2.180 (5)
Sn1–O1	2.276 (5)	Sn2–O7	2.226 (6)
Sn1–O5	2.203 (5)	Sn2–O3 <sup>i</sup>	2.246 (6)
C1–Sn1–C7	110.2 (2)	C19–Sn2–C25	124.6 (3)
C1–Sn1–C13	109.5 (2)	C19–Sn2–C31	122.9 (2)
C1–Sn1–O1	87.9 (2)	C19–Sn2–O3 <sup>i</sup>	89.9 (2)
C1–Sn1–O5	87.3 (2)	C19–Sn2–O7	91.0 (2)
C7–Sn1–C13	140.3 (2)	C25–Sn2–C31	112.5 (3)
C7–Sn1–O1	89.1 (2)	C25–Sn2–O3 <sup>i</sup>	85.8 (3)
C7–Sn1–O5	92.4 (2)	C25–Sn2–O7	91.7 (3)
C13–Sn1–O1	89.6 (2)	C31–Sn2–O3 <sup>i</sup>	95.2 (2)
C13–Sn1–O5	92.1 (2)	C31–Sn2–O7	86.4 (2)
O1–Sn1–O5	175.2 (2)	O3 <sup>i</sup> –Sn2–O7	177.4 (2)

Symmetry code: (i)  $x - 1, y - 1, z - 1$ .**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1n $\cdots$ O4	0.91	1.86	2.762 (9)	169
N2–H2n $\cdots$ O8	0.91	1.80	2.709 (10)	177

Phenyl rings were refined as rigid hexagons with 1.39 Å edges. There was some disorder in the cations, which was not resolved. For these, the C–N distances were restrained to 1.50 (1) Å and the C–C distances to 1.54 (1) Å; the N $\cdots$ C and C $\cdots$ C distances were restrained to 2.49 (1) Å and 2.45 (1) Å, respectively. The restraints ensured no short intramolecular H $\cdots$ H contacts of less than 2 Å except for only one contact (H50c $\cdots$ H53b) only. Additionally, all atoms in the structure were restrained to approximately isotropic behavior.