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catena-Poly[[trimethyltin(IV)]- μ -2-(2-chlorophenyl)acetato]

Liyuan Wen, Handong Yin* and Wenkuan Li

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: handongyin@163.com

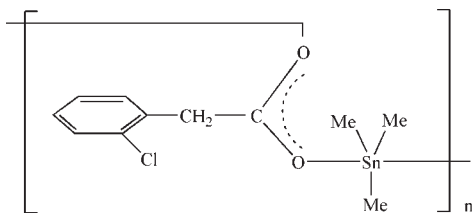
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.014$ Å; R factor = 0.047; wR factor = 0.107; data-to-parameter ratio = 17.4.

In the title polymeric coordination compound, $[\text{Sn}(\text{CH}_3)_3(\text{C}_8\text{H}_6\text{ClO}_2)]_n$, the Sn atoms exhibit a distorted trigonal-bipyramidal geometry with the carboxylate O atoms of the 2-chlorophenylacetato ligands in axial positions and with the equatorial sites occupied by the three methyl groups. Adjacent Sn atoms are bridged by coordination to the two O atoms of each 2-chlorophenylacetato ligand, forming a chain structure.

Related literature

For the biological activity of organotin compounds, see: Wang *et al.* (2007). For related structures, see: Wang *et al.* (2007); Ma *et al.* (2006).



Experimental

Crystal data

 $[\text{Sn}(\text{CH}_3)_3(\text{C}_8\text{H}_6\text{ClO}_2)]_n$ $M_r = 333.39$ Monoclinic, $P2_1/n$ $a = 7.0754$ (9) Å $b = 28.306$ (3) Å $c = 13.6721$ (15) Å $\beta = 93.117$ (2)° $V = 2734.1$ (5) Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 2.05$ mm⁻¹ $T = 298$ K $0.49 \times 0.32 \times 0.15$ mm

Data collection

Siemens SMART CCD area-

detector diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.434$, $T_{\max} = 0.749$

14063 measured reflections

4820 independent reflections

3411 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.056$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.047$ $wR(F^2) = 0.107$ $S = 1.05$

4820 reflections

277 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.09$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.92$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|---------|-----------|---------------------|-----------|
| Sn1—C17 | 2.107 (7) | Sn2—C22 | 2.102 (7) |
| Sn1—C18 | 2.117 (7) | Sn2—C20 | 2.113 (7) |
| Sn1—C19 | 2.120 (7) | Sn2—C21 | 2.117 (7) |
| Sn1—O3 | 2.194 (4) | Sn2—O2 | 2.207 (5) |
| Sn1—O1 | 2.396 (5) | Sn2—O4 ⁱ | 2.432 (5) |

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2651).

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supplementary materials

Acta Cryst. (2009). E65, m1261 [doi:10.1107/S1600536809038872]

catena-Poly[[trimethyltin(IV)]- μ -2-(2-chlorophenyl)acetato]

L. Wen, H. Yin and W. Li

Comment

The chemistry of organotin(IV) derivatives is a subject of study with growing interest due to their significant antimicrobial properties as well as antitumor activities (Wang *et al.*, 2007). As a part of our ongoing investigations in this field we have synthesized the title compound and present its crystal structure here. The title compound, which is shown in Fig.1 forms an extended one-dimensional chain structure arising from Sn—O bridges formed by the 2-(2-chlorophenyl)acetato ligands. The Sn—O bond distances in the compound (Sn(1)—O(1) = 2.396 (5) Å; Sn(1)—O(3) = 2.194 (4) Å) are comparable to those found in related organotin carboxylates (Ma *et al.*, 2006). The Sn atom assumes a slightly distorted trigonal-bipyramidal coordination geometry, provided by and three methyl groups in the equatorial positions and two O atoms of symmetry related carboxylate groups in the axial positions.

Experimental

The reaction was carried out under a nitrogen atmosphere. 2-(2-chlorophenyl)acetic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to a stirred solution of benzene (30 ml) in a Schlenk flask and stirred for 0.5 h. Trimethyltin chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 12 h at room temperature. The resulting clear solution was evaporated under vacuum. The product was crystallized from a solution of dichloromethane/methanol (1:1) to yield colourless blocks of the title compound (yield 81%. m.p.390 K). Anal. Calcd (%) for C₁₁H₁₅Cl₁O₂Sn₁ (Mr = 333.37): C,39.63; H, 4.54; Cl, 10.63. Found (%): C, 39.51; H, 4.64; Cl, 10.75.

Refinement

The H atoms were positioned geometrically, with methyl C—H distances of 0.96 Å and aromatic C—H distances of 0.93 Å, and refined as riding on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{O})$ or $1.5 U_{\text{eq}}(\text{C})$ for the methyl groups.

Figures

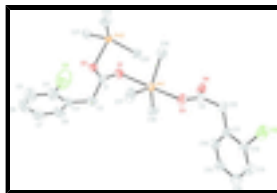


Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

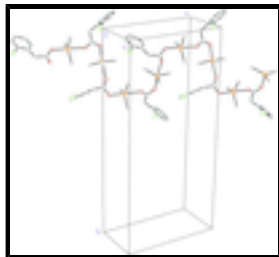


Fig. 2. A view of the one-dimensional extended chain structure in the title compound.

catena-Poly[[trimethyltin(IV)]- μ -2-(2-chlorophenyl)acetato]

Crystal data

[Sn(CH₃)₃(C₈H₆ClO₂)]

$M_r = 333.39$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.0754$ (9) Å

$b = 28.306$ (3) Å

$c = 13.6721$ (15) Å

$\beta = 93.117$ (2)°

$V = 2734.1$ (5) Å³

$Z = 8$

$F_{000} = 1312$

$D_x = 1.620$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4326 reflections

$\theta = 2.6$ – 24.8 °

$\mu = 2.05$ mm⁻¹

$T = 298$ K

Block, colourless

$0.49 \times 0.32 \times 0.15$ mm

Data collection

Siemens SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.434$, $T_{\max} = 0.749$

14063 measured reflections

4820 independent reflections

3411 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 25.0$ °

$\theta_{\min} = 1.7$ °

$h = -8 \rightarrow 8$

$k = -33 \rightarrow 33$

$l = -10 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.107$

$S = 1.05$

4820 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2 + 9.0463P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 1.09$ e Å⁻³

277 parameters

$$\Delta\rho_{\min} = -0.92 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|--------------|----------------------------------|
| Sn1 | 0.02624 (7) | 0.138217 (16) | 0.88059 (3) | 0.04764 (16) |
| Sn2 | 0.20583 (7) | 0.212967 (17) | 1.21572 (3) | 0.04848 (16) |
| Cl1 | 0.4073 (6) | 0.03321 (16) | 1.1310 (3) | 0.1655 (15) |
| Cl2 | -0.2267 (4) | 0.14040 (10) | 0.36127 (15) | 0.0943 (8) |
| O1 | 0.1070 (7) | 0.14009 (16) | 1.0530 (3) | 0.0583 (13) |
| O2 | 0.1197 (7) | 0.13802 (16) | 1.2145 (3) | 0.0572 (13) |
| O3 | -0.0431 (7) | 0.13733 (16) | 0.7223 (3) | 0.0564 (13) |
| O4 | -0.1907 (7) | 0.20535 (18) | 0.7318 (3) | 0.0620 (14) |
| C1 | 0.0842 (11) | 0.1192 (3) | 1.1319 (5) | 0.0553 (19) |
| C2 | 0.0044 (13) | 0.0697 (3) | 1.1322 (6) | 0.073 (2) |
| H2A | -0.1323 | 0.0720 | 1.1333 | 0.088* |
| H2B | 0.0328 | 0.0546 | 1.0710 | 0.088* |
| C3 | 0.0721 (17) | 0.0382 (3) | 1.2138 (7) | 0.079 (3) |
| C4 | 0.2486 (19) | 0.0191 (4) | 1.2200 (8) | 0.103 (3) |
| C5 | 0.316 (2) | -0.0112 (4) | 1.2941 (10) | 0.127 (4) |
| H5 | 0.4382 | -0.0237 | 1.2975 | 0.153* |
| C6 | 0.184 (3) | -0.0208 (4) | 1.3620 (10) | 0.121 (5) |
| H6 | 0.2224 | -0.0410 | 1.4131 | 0.145* |
| C7 | 0.001 (2) | -0.0036 (4) | 1.3623 (9) | 0.115 (4) |
| H7 | -0.0816 | -0.0121 | 1.4100 | 0.138* |
| C8 | -0.0504 (18) | 0.0264 (3) | 1.2880 (8) | 0.100 (3) |
| H8 | -0.1708 | 0.0397 | 1.2861 | 0.120* |
| C9 | -0.1339 (10) | 0.1720 (3) | 0.6832 (5) | 0.0504 (18) |
| C10 | -0.1744 (10) | 0.1690 (3) | 0.5734 (5) | 0.0553 (19) |
| H10A | -0.0690 | 0.1534 | 0.5443 | 0.066* |
| H10B | -0.1837 | 0.2007 | 0.5469 | 0.066* |
| C11 | -0.3557 (10) | 0.1423 (2) | 0.5447 (5) | 0.0514 (18) |
| C12 | -0.3923 (11) | 0.1278 (3) | 0.4478 (6) | 0.062 (2) |
| C13 | -0.5520 (14) | 0.1049 (3) | 0.4182 (7) | 0.079 (3) |
| H13 | -0.5713 | 0.0958 | 0.3531 | 0.095* |
| C14 | -0.6863 (13) | 0.0950 (3) | 0.4838 (7) | 0.080 (3) |
| H14 | -0.7967 | 0.0792 | 0.4633 | 0.097* |
| C15 | -0.6576 (12) | 0.1084 (3) | 0.5797 (7) | 0.072 (2) |
| H15 | -0.7488 | 0.1020 | 0.6244 | 0.086* |
| C16 | -0.4919 (11) | 0.1317 (3) | 0.6100 (6) | 0.064 (2) |
| H16 | -0.4723 | 0.1403 | 0.6754 | 0.077* |
| C17 | 0.1855 (13) | 0.0758 (3) | 0.8683 (6) | 0.079 (3) |
| H17A | 0.2891 | 0.0759 | 0.9167 | 0.119* |
| H17B | 0.2338 | 0.0741 | 0.8041 | 0.119* |
| H17C | 0.1062 | 0.0489 | 0.8785 | 0.119* |
| C18 | -0.2588 (11) | 0.1335 (3) | 0.9193 (6) | 0.077 (2) |

supplementary materials

| | | | | |
|------|--------------|------------|------------|-----------|
| H18A | -0.3086 | 0.1030 | 0.9012 | 0.115* |
| H18B | -0.3322 | 0.1576 | 0.8855 | 0.115* |
| H18C | -0.2649 | 0.1378 | 0.9887 | 0.115* |
| C19 | 0.1885 (11) | 0.2012 (3) | 0.8801 (5) | 0.069 (2) |
| H19A | 0.3035 | 0.1969 | 0.9196 | 0.103* |
| H19B | 0.1171 | 0.2266 | 0.9062 | 0.103* |
| H19C | 0.2183 | 0.2086 | 0.8141 | 0.103* |
| C20 | -0.0375 (10) | 0.2385 (3) | 1.1363 (6) | 0.067 (2) |
| H20A | -0.0001 | 0.2560 | 1.0803 | 0.100* |
| H20B | -0.1072 | 0.2588 | 1.1776 | 0.100* |
| H20C | -0.1158 | 0.2124 | 1.1149 | 0.100* |
| C21 | 0.2034 (13) | 0.2164 (3) | 1.3703 (5) | 0.075 (3) |
| H21A | 0.1478 | 0.2458 | 1.3891 | 0.112* |
| H21B | 0.3308 | 0.2145 | 1.3980 | 0.112* |
| H21C | 0.1306 | 0.1906 | 1.3939 | 0.112* |
| C22 | 0.4641 (10) | 0.2008 (3) | 1.1510 (6) | 0.071 (2) |
| H22A | 0.4750 | 0.1678 | 1.1356 | 0.107* |
| H22B | 0.5669 | 0.2099 | 1.1957 | 0.107* |
| H22C | 0.4684 | 0.2191 | 1.0920 | 0.107* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|------------|-------------|--------------|-------------|--------------|
| Sn1 | 0.0547 (3) | 0.0418 (3) | 0.0458 (3) | 0.0031 (2) | -0.0036 (2) | -0.0021 (2) |
| Sn2 | 0.0490 (3) | 0.0512 (3) | 0.0451 (3) | -0.0101 (2) | 0.0020 (2) | -0.0036 (2) |
| Cl1 | 0.138 (3) | 0.195 (4) | 0.163 (3) | 0.045 (3) | 0.005 (3) | 0.002 (3) |
| Cl2 | 0.1043 (18) | 0.130 (2) | 0.0492 (12) | -0.0172 (16) | 0.0086 (12) | -0.0131 (13) |
| O1 | 0.083 (4) | 0.046 (3) | 0.045 (3) | -0.007 (3) | -0.002 (2) | 0.000 (2) |
| O2 | 0.083 (4) | 0.047 (3) | 0.041 (3) | -0.015 (3) | -0.001 (2) | -0.003 (2) |
| O3 | 0.074 (3) | 0.049 (3) | 0.045 (3) | 0.017 (3) | -0.008 (2) | -0.007 (2) |
| O4 | 0.073 (4) | 0.058 (3) | 0.054 (3) | 0.022 (3) | -0.009 (3) | -0.005 (3) |
| C1 | 0.071 (5) | 0.046 (4) | 0.048 (4) | -0.003 (4) | -0.007 (4) | 0.001 (4) |
| C2 | 0.102 (7) | 0.057 (5) | 0.059 (5) | -0.019 (5) | -0.013 (5) | 0.001 (4) |
| C3 | 0.122 (9) | 0.044 (5) | 0.068 (6) | -0.019 (5) | -0.016 (6) | -0.006 (4) |
| C4 | 0.145 (11) | 0.071 (7) | 0.088 (7) | -0.001 (7) | -0.021 (8) | -0.002 (6) |
| C5 | 0.181 (14) | 0.084 (9) | 0.113 (10) | 0.012 (9) | -0.035 (10) | -0.006 (8) |
| C6 | 0.195 (16) | 0.064 (8) | 0.101 (10) | -0.014 (9) | -0.027 (10) | 0.006 (7) |
| C7 | 0.178 (14) | 0.078 (8) | 0.089 (8) | -0.040 (9) | -0.007 (9) | -0.002 (7) |
| C8 | 0.153 (10) | 0.060 (6) | 0.084 (7) | -0.026 (6) | -0.011 (7) | -0.003 (6) |
| C9 | 0.051 (4) | 0.057 (5) | 0.043 (4) | 0.007 (4) | -0.002 (3) | 0.001 (4) |
| C10 | 0.055 (5) | 0.063 (5) | 0.047 (4) | 0.003 (4) | -0.006 (3) | -0.001 (4) |
| C11 | 0.050 (4) | 0.053 (5) | 0.051 (4) | 0.007 (3) | -0.007 (3) | 0.000 (3) |
| C12 | 0.064 (5) | 0.061 (5) | 0.060 (5) | 0.002 (4) | -0.009 (4) | -0.010 (4) |
| C13 | 0.087 (7) | 0.074 (6) | 0.074 (6) | -0.010 (5) | -0.012 (5) | -0.010 (5) |
| C14 | 0.077 (6) | 0.068 (6) | 0.094 (7) | -0.012 (5) | -0.012 (5) | -0.002 (5) |
| C15 | 0.063 (5) | 0.070 (6) | 0.083 (6) | -0.010 (4) | 0.008 (5) | 0.005 (5) |
| C16 | 0.068 (5) | 0.066 (5) | 0.058 (5) | 0.000 (4) | 0.000 (4) | 0.000 (4) |
| C17 | 0.106 (7) | 0.071 (6) | 0.060 (5) | 0.036 (5) | -0.013 (5) | -0.009 (4) |

| | | | | | | |
|-----|-----------|-----------|-----------|------------|-----------|------------|
| C18 | 0.059 (5) | 0.093 (7) | 0.078 (6) | -0.008 (5) | 0.006 (4) | 0.006 (5) |
| C19 | 0.074 (5) | 0.075 (6) | 0.057 (5) | -0.017 (4) | 0.000 (4) | 0.012 (4) |
| C20 | 0.050 (5) | 0.063 (5) | 0.086 (6) | 0.003 (4) | 0.001 (4) | -0.010 (4) |
| C21 | 0.117 (7) | 0.068 (6) | 0.039 (4) | -0.029 (5) | 0.005 (4) | -0.004 (4) |
| C22 | 0.057 (5) | 0.082 (6) | 0.076 (5) | -0.006 (4) | 0.006 (4) | -0.003 (5) |

Geometric parameters (Å, °)

| | | | |
|----------------------|------------|---------------|------------|
| Sn1—C17 | 2.107 (7) | C10—C11 | 1.522 (9) |
| Sn1—C18 | 2.117 (7) | C10—H10A | 0.9700 |
| Sn1—C19 | 2.120 (7) | C10—H10B | 0.9700 |
| Sn1—O3 | 2.194 (4) | C11—C16 | 1.381 (10) |
| Sn1—O1 | 2.396 (5) | C11—C12 | 1.397 (10) |
| Sn2—C22 | 2.102 (7) | C12—C13 | 1.345 (11) |
| Sn2—C20 | 2.113 (7) | C13—C14 | 1.371 (12) |
| Sn2—C21 | 2.117 (7) | C13—H13 | 0.9300 |
| Sn2—O2 | 2.207 (5) | C14—C15 | 1.369 (11) |
| Sn2—O4 ⁱ | 2.432 (5) | C14—H14 | 0.9300 |
| C11—C4 | 1.746 (12) | C15—C16 | 1.389 (11) |
| C12—C12 | 1.747 (8) | C15—H15 | 0.9300 |
| O1—C1 | 1.249 (8) | C16—H16 | 0.9300 |
| O2—C1 | 1.263 (8) | C17—H17A | 0.9600 |
| O3—C9 | 1.273 (8) | C17—H17B | 0.9600 |
| O4—C9 | 1.235 (8) | C17—H17C | 0.9600 |
| O4—Sn2 ⁱⁱ | 2.432 (5) | C18—H18A | 0.9600 |
| C1—C2 | 1.510 (10) | C18—H18B | 0.9600 |
| C2—C3 | 1.487 (11) | C18—H18C | 0.9600 |
| C2—H2A | 0.9700 | C19—H19A | 0.9600 |
| C2—H2B | 0.9700 | C19—H19B | 0.9600 |
| C3—C4 | 1.359 (14) | C19—H19C | 0.9600 |
| C3—C8 | 1.411 (13) | C20—H20A | 0.9600 |
| C4—C5 | 1.395 (15) | C20—H20B | 0.9600 |
| C5—C6 | 1.380 (17) | C20—H20C | 0.9600 |
| C5—H5 | 0.9300 | C21—H21A | 0.9600 |
| C6—C7 | 1.387 (17) | C21—H21B | 0.9600 |
| C6—H6 | 0.9300 | C21—H21C | 0.9600 |
| C7—C8 | 1.358 (14) | C22—H22A | 0.9600 |
| C7—H7 | 0.9300 | C22—H22B | 0.9600 |
| C8—H8 | 0.9300 | C22—H22C | 0.9600 |
| C9—C10 | 1.515 (9) | | |
| C17—Sn1—C18 | 119.2 (4) | C9—C10—H10B | 108.9 |
| C17—Sn1—C19 | 114.4 (4) | C11—C10—H10B | 108.9 |
| C18—Sn1—C19 | 125.2 (3) | H10A—C10—H10B | 107.7 |
| C17—Sn1—O3 | 90.2 (2) | C16—C11—C12 | 116.7 (7) |
| C18—Sn1—O3 | 94.6 (3) | C16—C11—C10 | 123.3 (6) |
| C19—Sn1—O3 | 95.6 (2) | C12—C11—C10 | 120.0 (7) |
| C17—Sn1—O1 | 89.8 (2) | C13—C12—C11 | 122.4 (8) |
| C18—Sn1—O1 | 86.3 (3) | C13—C12—C12 | 118.5 (7) |

supplementary materials

| | | | |
|-------------------------|-------------|---------------|-----------|
| C19—Sn1—O1 | 83.4 (2) | C11—C12—C12 | 119.1 (6) |
| O3—Sn1—O1 | 178.93 (18) | C12—C13—C14 | 120.1 (8) |
| C22—Sn2—C20 | 122.9 (3) | C12—C13—H13 | 119.9 |
| C22—Sn2—C21 | 118.9 (3) | C14—C13—H13 | 119.9 |
| C20—Sn2—C21 | 116.5 (3) | C15—C14—C13 | 119.9 (8) |
| C22—Sn2—O2 | 94.9 (3) | C15—C14—H14 | 120.1 |
| C20—Sn2—O2 | 96.2 (3) | C13—C14—H14 | 120.1 |
| C21—Sn2—O2 | 92.0 (2) | C14—C15—C16 | 119.7 (8) |
| C22—Sn2—O4 ⁱ | 86.0 (3) | C14—C15—H15 | 120.1 |
| C20—Sn2—O4 ⁱ | 87.3 (2) | C16—C15—H15 | 120.1 |
| C21—Sn2—O4 ⁱ | 83.4 (2) | C11—C16—C15 | 121.2 (7) |
| O2—Sn2—O4 ⁱ | 175.08 (16) | C11—C16—H16 | 119.4 |
| C1—O1—Sn1 | 143.5 (5) | C15—C16—H16 | 119.4 |
| C1—O2—Sn2 | 117.0 (4) | Sn1—C17—H17A | 109.5 |
| C9—O3—Sn1 | 119.0 (4) | Sn1—C17—H17B | 109.5 |
| C9—O4—Sn2 ⁱⁱ | 141.7 (5) | H17A—C17—H17B | 109.5 |
| O1—C1—O2 | 122.9 (7) | Sn1—C17—H17C | 109.5 |
| O1—C1—C2 | 120.6 (6) | H17A—C17—H17C | 109.5 |
| O2—C1—C2 | 116.5 (6) | H17B—C17—H17C | 109.5 |
| C3—C2—C1 | 116.9 (7) | Sn1—C18—H18A | 109.5 |
| C3—C2—H2A | 108.1 | Sn1—C18—H18B | 109.5 |
| C1—C2—H2A | 108.1 | H18A—C18—H18B | 109.5 |
| C3—C2—H2B | 108.1 | Sn1—C18—H18C | 109.5 |
| C1—C2—H2B | 108.1 | H18A—C18—H18C | 109.5 |
| H2A—C2—H2B | 107.3 | H18B—C18—H18C | 109.5 |
| C4—C3—C8 | 117.4 (10) | Sn1—C19—H19A | 109.5 |
| C4—C3—C2 | 122.9 (10) | Sn1—C19—H19B | 109.5 |
| C8—C3—C2 | 119.8 (10) | H19A—C19—H19B | 109.5 |
| C3—C4—C5 | 124.7 (13) | Sn1—C19—H19C | 109.5 |
| C3—C4—C11 | 119.3 (9) | H19A—C19—H19C | 109.5 |
| C5—C4—C11 | 116.0 (12) | H19B—C19—H19C | 109.5 |
| C6—C5—C4 | 113.0 (14) | Sn2—C20—H20A | 109.5 |
| C6—C5—H5 | 123.5 | Sn2—C20—H20B | 109.5 |
| C4—C5—H5 | 123.5 | H20A—C20—H20B | 109.5 |
| C5—C6—C7 | 127.0 (13) | Sn2—C20—H20C | 109.5 |
| C5—C6—H6 | 116.5 | H20A—C20—H20C | 109.5 |
| C7—C6—H6 | 116.5 | H20B—C20—H20C | 109.5 |
| C8—C7—C6 | 115.4 (13) | Sn2—C21—H21A | 109.5 |
| C8—C7—H7 | 122.3 | Sn2—C21—H21B | 109.5 |
| C6—C7—H7 | 122.3 | H21A—C21—H21B | 109.5 |
| C7—C8—C3 | 122.5 (12) | Sn2—C21—H21C | 109.5 |
| C7—C8—H8 | 118.8 | H21A—C21—H21C | 109.5 |
| C3—C8—H8 | 118.8 | H21B—C21—H21C | 109.5 |
| O4—C9—O3 | 122.4 (6) | Sn2—C22—H22A | 109.5 |
| O4—C9—C10 | 121.7 (6) | Sn2—C22—H22B | 109.5 |
| O3—C9—C10 | 115.9 (6) | H22A—C22—H22B | 109.5 |
| C9—C10—C11 | 113.2 (6) | Sn2—C22—H22C | 109.5 |
| C9—C10—H10A | 108.9 | H22A—C22—H22C | 109.5 |

| | | | |
|----------------------------|------------|------------------------------|------------|
| C11—C10—H10A | 108.9 | H22B—C22—H22C | 109.5 |
| C17—Sn1—O1—C1 | -67.1 (9) | C11—C4—C5—C6 | 179.9 (9) |
| C18—Sn1—O1—C1 | 52.3 (9) | C4—C5—C6—C7 | -0.1 (19) |
| C19—Sn1—O1—C1 | 178.4 (9) | C5—C6—C7—C8 | -1.2 (19) |
| O3—Sn1—O1—C1 | -159 (9) | C6—C7—C8—C3 | 2.0 (15) |
| C22—Sn2—O2—C1 | -66.8 (6) | C4—C3—C8—C7 | -1.6 (14) |
| C20—Sn2—O2—C1 | 57.1 (6) | C2—C3—C8—C7 | 177.3 (8) |
| C21—Sn2—O2—C1 | 174.0 (6) | Sn2 ⁱⁱ —O4—C9—O3 | 160.1 (5) |
| O4 ⁱ —Sn2—O2—C1 | -167 (2) | Sn2 ⁱⁱ —O4—C9—C10 | -22.1 (12) |
| C17—Sn1—O3—C9 | -174.5 (6) | Sn1—O3—C9—O4 | -2.7 (9) |
| C18—Sn1—O3—C9 | 66.2 (6) | Sn1—O3—C9—C10 | 179.3 (4) |
| C19—Sn1—O3—C9 | -60.0 (6) | O4—C9—C10—C11 | -91.2 (9) |
| O1—Sn1—O3—C9 | -83 (10) | O3—C9—C10—C11 | 86.7 (8) |
| Sn1—O1—C1—O2 | -163.3 (5) | C9—C10—C11—C16 | 14.6 (10) |
| Sn1—O1—C1—C2 | 14.4 (13) | C9—C10—C11—C12 | -166.5 (7) |
| Sn2—O2—C1—O1 | 4.5 (10) | C16—C11—C12—C13 | 0.3 (11) |
| Sn2—O2—C1—C2 | -173.3 (5) | C10—C11—C12—C13 | -178.7 (8) |
| O1—C1—C2—C3 | 148.0 (8) | C16—C11—C12—C12 | 179.6 (6) |
| O2—C1—C2—C3 | -34.2 (11) | C10—C11—C12—C12 | 0.6 (10) |
| C1—C2—C3—C4 | -72.9 (11) | C11—C12—C13—C14 | 0.1 (13) |
| C1—C2—C3—C8 | 108.2 (9) | C12—C12—C13—C14 | -179.1 (7) |
| C8—C3—C4—C5 | 0.2 (15) | C12—C13—C14—C15 | -0.1 (14) |
| C2—C3—C4—C5 | -178.7 (9) | C13—C14—C15—C16 | -0.4 (13) |
| C8—C3—C4—C11 | -179.1 (7) | C12—C11—C16—C15 | -0.8 (11) |
| C2—C3—C4—C11 | 2.0 (13) | C10—C11—C16—C15 | 178.1 (7) |
| C3—C4—C5—C6 | 0.6 (17) | C14—C15—C16—C11 | 0.9 (12) |

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $x-1/2, -y+1/2, z-1/2$.

Fig. 1

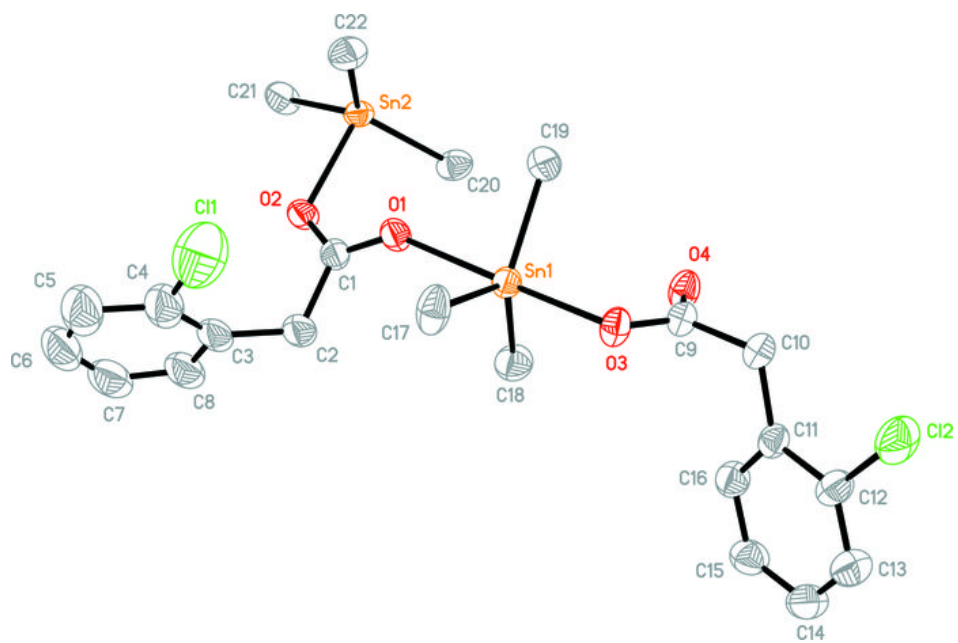


Fig. 2

