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(5-Bromosalicylato)triphenyltin(IV)

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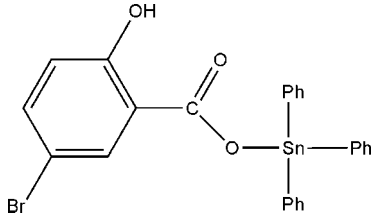
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.014 Å; R factor = 0.050; wR factor = 0.104; data-to-parameter ratio = 14.6.

The title compound, $[Sn(C_6H_5)_3(C_7H_4BrO_3)]$, crystallizes with two independent molecules in the asymmetric unit, the molecular conformations of which are almost identical. In each molecule, the Sn atom is coordinated by one O and three C atoms in a distorted tetrahedral geometry [Sn—O = 2.045 (4) and 2.087 (4) Å; Sn—C = 2.082 (7)–2.117 (7)Å]. The hydroxy groups are involved in intramolecular O—H···O hydrogen bonds.

Related literature

A series of new triorganotin(IV) pyridinedicarboxylates has been synthesized by the reaction of trimethyltin(IV), triphenyltin(IV) or tribenzyltin(IV) chloride with 2,6(3,5 or 2,5)-H_2pdc (pdc = pyridinedicarboxylate), see: Ma *et al.* (2006).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_7H_4BrO_3)]$
M_r = 566.00
Triclinic, $P\overline{1}$
a = 11.434 (7) Å
b = 14.233 (9) Å
c = 15.453 (10) Å
α = 113.920 (7)°
β = 92.418 (8)°
γ = 93.818 (9)°
V = 2287 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.89 mm^{-1}
T = 298 (2) K
0.52 × 0.47 × 0.41 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.315, T_{max} = 0.384
(expected range = 0.251–0.306)
11810 measured reflections
7898 independent reflections
4460 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.104
S = 1.00
7898 reflections
541 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.49 e Å^{-3}
$\Delta\rho_{min}$ = −1.08 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	1.86	2.583 (8)	146
O6—H6···O5	0.82	1.86	2.583 (9)	147

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: CV2335).

References

Ma, C., Li, J., Zhang, R. & Wang, D. (2006). *J. Organomet. Chem.* **691**, 1713–1721.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

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(5-Bromosalicylato)triphenyltin(IV)

H. Wang, H. Yin and D. Wang

Comment

Organotin esters of carboxylic acids are widely used as biocides, as fungicides and in industry as homogeneous catalysts. We have therefore synthesized the title compound, (I), and present its crystal structure here.

In (I) (Fig. 1), the tin atoms are four-coordinated by the three C atoms from phenyls and the oxygen atom of the monodentate carboxyl group. Thus, the geometry of the tin centers displays a distorted tetrahedral coordinated sphere with six angles ranging from 95.2 (2) ° to 125.0 (3) °. The Sn1—O1 distance of 2.045 (4) Å is close to the reported values for triorganotin carboxylates (Ma *et al.*, 2006).

Experimental

The reaction was carried out under nitrogen atmosphere. 5-Bromosalicylic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to the solution of benzene in a Schlenk flask and stirred for 0.5 h. Triphenyltin chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 12 h at 313 K. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1) (yield 80%; m.p. 427 K). Analysis, calculated (%) for $C_{25}H_{19}BrO_3Sn$ (Mr = 566.00): C, 53.05; H, 3.39. found: C, 53.36; H, 3.23.

Refinement

H atoms were positioned geometrically, with O—H =0.82 Å and C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*O*) The residual peak of 1.49 e Å^3 situated 0.45 Å at atom Br2.

Figures

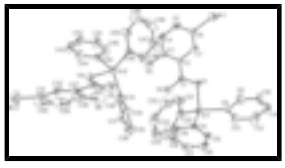


Fig. 1. The content of asymmetric unit of (I), with atomic numbering and 50% probability displacement ellipsoids for non-H atoms.

(5-Bromosalicylato)triphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_7H_4BrO_3)]$	Z = 4
M_r = 566.00	F_{000} = 1112
Triclinic, $P\bar{1}$	D_x = 1.644 Mg m^{-3}
a = 11.434 (7) Å	Mo $K\alpha$ radiation

	λ = 0.71073 Å
b = 14.233 (9) Å	Cell parameters from 2851 reflections
c = 15.453 (10) Å	θ = 2.4–22.2º
α = 113.920 (7)º	μ = 2.89 mm^{-1}
β = 92.418 (8)º	*T* = 298 (2) K
γ = 93.818 (9)º	Block, colourless
V = 2287 (3) Å^3	0.52 × 0.47 × 0.41 mm

Data collection

Bruker SMART CCD area-detector diffractometer	7898 independent reflections
Radiation source: fine-focus sealed tube	4460 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 298(2) K	θ_{max} = 25.0º
phi and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −8→13
T_{min} = 0.315, T_{max} = 0.384	*k* = −16→16
11810 measured reflections	*l* = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
7898 reflections	$\Delta\rho_{max}$ = 1.49 e Å^{-3}
541 parameters	$\Delta\rho_{min}$ = −1.08 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.73602 (4)	0.56543 (3)	0.32221 (3)	0.04496 (16)
Sn2	0.84682 (4)	0.90686 (4)	0.12077 (3)	0.04421 (16)
O1	0.7057 (4)	0.5070 (3)	0.1778 (3)	0.0520 (12)
O2	0.6858 (4)	0.6686 (4)	0.1996 (3)	0.0572 (13)
O3	0.6488 (4)	0.7113 (3)	0.0540 (3)	0.0632 (14)
H3	0.6599	0.7239	0.1105	0.095*
O4	0.9747 (4)	1.0319 (3)	0.1780 (3)	0.0536 (13)
O5	1.0545 (4)	0.9425 (4)	0.2486 (4)	0.0734 (16)
O6	1.2595 (6)	1.0097 (6)	0.3379 (5)	0.122 (3)

H6	1.2034	0.9675	0.3105	0.183*
Br1	0.63956 (9)	0.25806 (6)	−0.18809 (6)	0.0788 (3)
Br2	1.19838 (15)	1.41108 (11)	0.30941 (9)	0.1746 (7)
C1	0.6843 (6)	0.5753 (6)	0.1463 (5)	0.0467 (18)
C2	0.6638 (5)	0.5393 (5)	0.0428 (5)	0.0411 (17)
C3	0.6493 (6)	0.6095 (6)	0.0026 (5)	0.0518 (19)
C4	0.6349 (7)	0.5739 (6)	−0.0959 (6)	0.066 (2)
H4	0.6281	0.6204	−0.1238	0.079*
C5	0.6308 (7)	0.4693 (6)	−0.1519 (5)	0.064 (2)
H5	0.6194	0.4453	−0.2176	0.077*
C6	0.6433 (6)	0.4013 (5)	−0.1114 (5)	0.0469 (18)
C7	0.6595 (5)	0.4357 (5)	−0.0149 (5)	0.0478 (18)
H7	0.6677	0.3886	0.0120	0.057*
C8	0.7657 (6)	0.4229 (5)	0.3271 (5)	0.0499 (19)
C9	0.7073 (8)	0.3321 (6)	0.2696 (6)	0.089 (3)
H9	0.6496	0.3315	0.2251	0.107*
C10	0.7293 (12)	0.2403 (6)	0.2739 (7)	0.123 (4)
H10	0.6870	0.1790	0.2332	0.148*
C11	0.8125 (11)	0.2406 (8)	0.3374 (8)	0.102 (4)
H11	0.8268	0.1790	0.3417	0.122*
C12	0.8754 (8)	0.3279 (8)	0.3948 (8)	0.095 (3)
H12	0.9348	0.3265	0.4370	0.114*
C13	0.8525 (7)	0.4185 (6)	0.3914 (6)	0.070 (2)
H13	0.8955	0.4791	0.4327	0.084*
C14	0.5805 (6)	0.6271 (5)	0.3818 (4)	0.0397 (17)
C15	0.5098 (7)	0.5749 (5)	0.4219 (5)	0.054 (2)
H15	0.5290	0.5120	0.4207	0.064*
C16	0.4100 (7)	0.6182 (7)	0.4639 (5)	0.070 (2)
H16	0.3625	0.5843	0.4917	0.084*
C17	0.3814 (7)	0.7104 (8)	0.4645 (5)	0.072 (2)
H17	0.3145	0.7389	0.4925	0.086*
C18	0.4490 (7)	0.7589 (6)	0.4251 (5)	0.061 (2)
H18	0.4285	0.8211	0.4254	0.073*
C19	0.5483 (6)	0.7192 (5)	0.3841 (5)	0.0512 (19)
H19	0.5947	0.7551	0.3574	0.061*
C20	0.8909 (6)	0.6673 (6)	0.3631 (5)	0.0533 (19)
C21	0.9877 (8)	0.6457 (7)	0.3116 (6)	0.079 (3)
H21	0.9842	0.5852	0.2566	0.095*
C22	1.0898 (8)	0.7106 (9)	0.3383 (7)	0.099 (3)
H22	1.1556	0.6924	0.3038	0.118*
C23	1.0931 (8)	0.8006 (8)	0.4151 (8)	0.083 (3)
H23	1.1602	0.8467	0.4309	0.099*
C24	1.0017 (9)	0.8253 (7)	0.4694 (7)	0.084 (3)
H24	1.0072	0.8865	0.5239	0.101*
C25	0.8973 (7)	0.7585 (6)	0.4437 (6)	0.067 (2)
H25	0.8334	0.7756	0.4806	0.080*
C26	1.0539 (6)	1.0204 (7)	0.2325 (5)	0.056 (2)
C27	1.1469 (6)	1.1072 (7)	0.2778 (5)	0.062 (2)
C28	1.2458 (8)	1.0956 (9)	0.3280 (6)	0.085 (3)

C29	1.3333 (12)	1.1784 (11)	0.3673 (9)	0.129 (6)
H29	1.4011	1.1718	0.3990	0.155*
C30	1.3190 (12)	1.2661 (13)	0.3590 (9)	0.144 (7)
H30	1.3782	1.3200	0.3854	0.173*
C31	1.2216 (10)	1.2814 (8)	0.3137 (6)	0.107 (4)
C32	1.1341 (7)	1.2010 (7)	0.2719 (5)	0.074 (3)
H32	1.0676	1.2096	0.2402	0.089*
C33	0.7522 (6)	0.9299 (5)	0.2414 (5)	0.0499 (19)
C34	0.8015 (7)	0.9261 (5)	0.3224 (5)	0.062 (2)
H34	0.8773	0.9062	0.3230	0.075*
C35	0.7407 (10)	0.9510 (6)	0.4028 (6)	0.082 (3)
H35	0.7762	0.9497	0.4575	0.098*
C36	0.6303 (11)	0.9772 (7)	0.4019 (8)	0.097 (4)
H36	0.5898	0.9944	0.4564	0.116*
C37	0.5765 (9)	0.9790 (7)	0.3219 (9)	0.104 (4)
H37	0.4990	0.9949	0.3211	0.124*
C38	0.6395 (7)	0.9566 (6)	0.2412 (6)	0.072 (2)
H38	0.6046	0.9600	0.1872	0.087*
C39	0.7617 (6)	0.9608 (5)	0.0278 (4)	0.0469 (18)
C40	0.6655 (8)	0.9063 (7)	−0.0313 (6)	0.087 (3)
H40	0.6358	0.8444	−0.0302	0.104*
C41	0.6120 (8)	0.9415 (8)	−0.0922 (7)	0.103 (3)
H41	0.5470	0.9030	−0.1319	0.124*
C42	0.6530 (8)	1.0315 (8)	−0.0950 (6)	0.085 (3)
H42	0.6158	1.0554	−0.1358	0.102*
C43	0.7477 (8)	1.0857 (7)	−0.0385 (7)	0.091 (3)
H43	0.7768	1.1474	−0.0403	0.110*
C44	0.8026 (7)	1.0501 (6)	0.0228 (6)	0.079 (3)
H44	0.8687	1.0883	0.0612	0.095*
C45	0.9356 (6)	0.7777 (5)	0.0486 (5)	0.0478 (18)
C46	0.9812 (7)	0.7202 (6)	0.0937 (6)	0.076 (2)
H46	0.9700	0.7381	0.1575	0.091*
C47	1.0421 (9)	0.6379 (7)	0.0463 (8)	0.101 (3)
H47	1.0719	0.5997	0.0774	0.121*
C48	1.0587 (8)	0.6121 (7)	−0.0455 (9)	0.104 (4)
H48	1.1013	0.5563	−0.0776	0.125*
C49	1.0150 (8)	0.6655 (8)	−0.0921 (7)	0.110 (4)
H49	1.0271	0.6468	−0.1559	0.132*
C50	0.9517 (6)	0.7488 (6)	−0.0443 (6)	0.069 (2)
H50	0.9200	0.7851	−0.0766	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0528 (3)	0.0453 (3)	0.0366 (3)	−0.0001 (3)	−0.0015 (2)	0.0178 (2)
Sn2	0.0393 (3)	0.0503 (3)	0.0422 (3)	0.0039 (2)	−0.0069 (2)	0.0191 (2)
O1	0.071 (3)	0.050 (3)	0.038 (3)	0.010 (3)	0.001 (2)	0.020 (2)
O2	0.072 (4)	0.054 (3)	0.042 (3)	0.001 (3)	0.000 (3)	0.017 (3)

O3	0.078 (4)	0.056 (3)	0.064 (4)	0.013 (3)	0.008 (3)	0.032 (3)
O4	0.043 (3)	0.062 (3)	0.050 (3)	−0.013 (3)	−0.018 (2)	0.022 (3)
O5	0.062 (4)	0.092 (4)	0.071 (4)	0.007 (3)	−0.009 (3)	0.040 (3)
O6	0.090 (5)	0.179 (8)	0.080 (5)	0.020 (5)	−0.037 (4)	0.038 (5)
Br1	0.1071 (7)	0.0675 (5)	0.0490 (5)	−0.0003 (5)	−0.0052 (5)	0.0131 (4)
Br2	0.2350 (17)	0.1388 (11)	0.1236 (11)	−0.1209 (12)	−0.0456 (10)	0.0531 (9)
C1	0.048 (5)	0.051 (5)	0.043 (5)	−0.001 (4)	0.011 (4)	0.022 (4)
C2	0.039 (4)	0.052 (4)	0.037 (4)	0.000 (4)	0.002 (3)	0.024 (4)
C3	0.054 (5)	0.060 (5)	0.046 (5)	0.000 (4)	0.004 (4)	0.026 (4)
C4	0.084 (6)	0.076 (6)	0.057 (6)	0.014 (5)	0.005 (5)	0.046 (5)
C5	0.077 (6)	0.080 (6)	0.035 (5)	0.000 (5)	−0.001 (4)	0.024 (5)
C6	0.043 (4)	0.050 (4)	0.050 (5)	−0.005 (4)	−0.005 (4)	0.025 (4)
C7	0.050 (5)	0.062 (5)	0.038 (4)	0.005 (4)	0.002 (3)	0.028 (4)
C8	0.069 (5)	0.045 (4)	0.037 (4)	0.002 (4)	0.008 (4)	0.018 (4)
C9	0.128 (8)	0.054 (5)	0.080 (7)	−0.005 (6)	−0.035 (6)	0.028 (5)
C10	0.230 (14)	0.036 (5)	0.099 (9)	0.012 (7)	−0.017 (9)	0.028 (6)
C11	0.149 (11)	0.080 (8)	0.109 (10)	0.051 (8)	0.047 (8)	0.062 (7)
C12	0.093 (8)	0.095 (7)	0.126 (9)	0.014 (7)	−0.007 (6)	0.074 (7)
C13	0.070 (6)	0.061 (5)	0.093 (7)	−0.002 (5)	−0.004 (5)	0.049 (5)
C14	0.042 (4)	0.048 (4)	0.029 (4)	0.000 (4)	−0.005 (3)	0.018 (3)
C15	0.060 (5)	0.060 (5)	0.040 (5)	−0.010 (4)	−0.007 (4)	0.024 (4)
C16	0.047 (5)	0.112 (8)	0.064 (6)	−0.014 (5)	0.005 (4)	0.053 (6)
C17	0.046 (5)	0.113 (8)	0.049 (5)	0.021 (6)	−0.003 (4)	0.025 (5)
C18	0.065 (6)	0.073 (6)	0.050 (5)	0.017 (5)	0.006 (4)	0.029 (4)
C19	0.054 (5)	0.052 (5)	0.044 (5)	−0.006 (4)	0.006 (4)	0.018 (4)
C20	0.046 (5)	0.069 (5)	0.051 (5)	−0.001 (4)	−0.006 (4)	0.033 (4)
C21	0.065 (6)	0.097 (7)	0.060 (6)	0.001 (6)	0.003 (5)	0.019 (5)
C22	0.056 (7)	0.134 (9)	0.096 (8)	−0.010 (7)	0.015 (6)	0.038 (7)
C23	0.059 (7)	0.090 (8)	0.114 (9)	−0.020 (6)	−0.017 (6)	0.064 (7)
C24	0.087 (7)	0.062 (6)	0.088 (7)	−0.007 (6)	−0.024 (6)	0.020 (5)
C25	0.052 (5)	0.066 (5)	0.071 (6)	0.002 (5)	0.001 (4)	0.018 (5)
C26	0.039 (5)	0.080 (6)	0.036 (5)	−0.009 (5)	0.003 (4)	0.013 (4)
C27	0.043 (5)	0.099 (7)	0.030 (4)	−0.008 (5)	−0.003 (4)	0.015 (5)
C28	0.051 (6)	0.142 (10)	0.043 (6)	0.008 (7)	−0.007 (4)	0.018 (6)
C29	0.062 (8)	0.207 (16)	0.062 (7)	−0.005 (11)	−0.026 (6)	0.003 (10)
C30	0.072 (10)	0.237 (18)	0.057 (8)	−0.067 (12)	−0.010 (6)	0.005 (11)
C31	0.117 (9)	0.132 (9)	0.044 (6)	−0.073 (8)	−0.017 (6)	0.021 (6)
C32	0.069 (6)	0.100 (7)	0.040 (5)	−0.034 (6)	−0.009 (4)	0.022 (5)
C33	0.047 (5)	0.034 (4)	0.054 (5)	−0.005 (4)	−0.012 (4)	0.006 (4)
C34	0.066 (6)	0.070 (5)	0.054 (5)	0.009 (5)	0.009 (5)	0.027 (4)
C35	0.105 (8)	0.072 (6)	0.059 (6)	−0.010 (6)	0.023 (6)	0.019 (5)
C36	0.114 (10)	0.063 (6)	0.087 (8)	−0.012 (7)	0.049 (7)	0.004 (6)
C37	0.061 (7)	0.080 (7)	0.147 (11)	0.008 (6)	0.054 (8)	0.019 (8)
C38	0.058 (6)	0.061 (5)	0.090 (7)	0.004 (5)	0.003 (5)	0.024 (5)
C39	0.046 (5)	0.054 (4)	0.041 (4)	0.003 (4)	−0.007 (4)	0.020 (4)
C40	0.090 (7)	0.082 (6)	0.095 (7)	−0.017 (6)	−0.041 (6)	0.052 (6)
C41	0.089 (8)	0.099 (8)	0.116 (9)	−0.038 (6)	−0.042 (6)	0.050 (7)
C42	0.078 (7)	0.117 (8)	0.079 (7)	−0.005 (6)	−0.015 (5)	0.065 (6)
C43	0.098 (8)	0.093 (7)	0.107 (8)	−0.012 (6)	−0.025 (6)	0.070 (6)

C44	0.078 (6)	0.085 (6)	0.084 (7)	−0.020 (5)	−0.031 (5)	0.051 (5)
C45	0.043 (4)	0.047 (4)	0.043 (5)	−0.002 (4)	0.002 (4)	0.009 (4)
C46	0.082 (6)	0.069 (6)	0.076 (6)	0.026 (5)	−0.005 (5)	0.028 (5)
C47	0.113 (8)	0.072 (7)	0.098 (8)	0.026 (6)	−0.030 (7)	0.016 (6)
C48	0.062 (6)	0.089 (7)	0.111 (10)	0.036 (5)	−0.017 (6)	−0.012 (7)
C49	0.083 (7)	0.147 (10)	0.062 (7)	0.034 (7)	0.012 (6)	0.001 (7)
C50	0.059 (5)	0.076 (6)	0.063 (6)	0.015 (5)	0.008 (4)	0.017 (5)

Geometric parameters (Å, °)

Sn1—O1	2.045 (4)	C21—C22	1.376 (11)
Sn1—C8	2.110 (7)	C21—H21	0.9300
Sn1—C20	2.112 (7)	C22—C23	1.344 (11)
Sn1—C14	2.115 (7)	C22—H22	0.9300
Sn2—C45	2.082 (7)	C23—C24	1.344 (11)
Sn2—O4	2.087 (4)	C23—H23	0.9300
Sn2—C33	2.116 (7)	C24—C25	1.411 (10)
Sn2—C39	2.117 (7)	C24—H24	0.9300
O1—C1	1.283 (7)	C25—H25	0.9300
O2—C1	1.246 (7)	C26—C27	1.486 (10)
O3—C3	1.340 (7)	C27—C32	1.390 (10)
O3—H3	0.8200	C27—C28	1.401 (11)
O4—C26	1.274 (8)	C28—C29	1.404 (15)
O5—C26	1.231 (8)	C29—C30	1.325 (17)
O6—C28	1.311 (11)	C29—H29	0.9300
O6—H6	0.8200	C30—C31	1.366 (16)
Br1—C6	1.894 (7)	C30—H30	0.9300
Br2—C31	1.910 (11)	C31—C32	1.386 (11)
C1—C2	1.470 (9)	C32—H32	0.9300
C2—C7	1.375 (8)	C33—C38	1.368 (10)
C2—C3	1.390 (9)	C33—C34	1.373 (9)
C3—C4	1.394 (9)	C34—C35	1.379 (10)
C4—C5	1.383 (9)	C34—H34	0.9300
C4—H4	0.9300	C35—C36	1.341 (12)
C5—C6	1.361 (9)	C35—H35	0.9300
C5—H5	0.9300	C36—C37	1.368 (13)
C6—C7	1.366 (8)	C36—H36	0.9300
C7—H7	0.9300	C37—C38	1.400 (11)
C8—C9	1.344 (9)	C37—H37	0.9300
C8—C13	1.396 (9)	C38—H38	0.9300
C9—C10	1.374 (11)	C39—C44	1.358 (9)
C9—H9	0.9300	C39—C40	1.368 (9)
C10—C11	1.336 (13)	C40—C41	1.372 (10)
C10—H10	0.9300	C40—H40	0.9300
C11—C12	1.334 (12)	C41—C42	1.353 (10)
C11—H11	0.9300	C41—H41	0.9300
C12—C13	1.354 (10)	C42—C43	1.340 (10)
C12—H12	0.9300	C42—H42	0.9300
C13—H13	0.9300	C43—C44	1.388 (10)

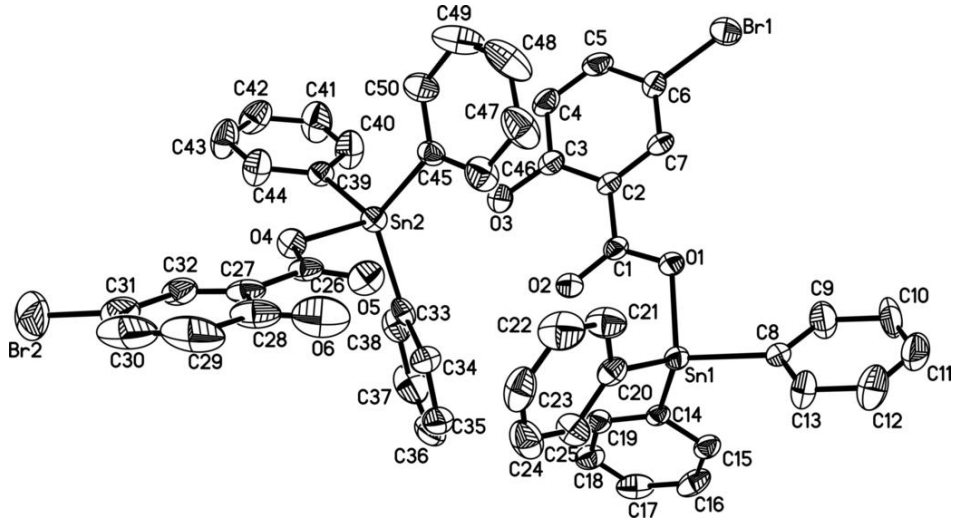
C14—C19	1.372 (8)	C43—H43	0.9300
C14—C15	1.387 (8)	C44—H44	0.9300
C15—C16	1.391 (10)	C45—C50	1.348 (9)
C15—H15	0.9300	C45—C46	1.384 (9)
C16—C17	1.370 (10)	C46—C47	1.360 (11)
C16—H16	0.9300	C46—H46	0.9300
C17—C18	1.324 (10)	C47—C48	1.339 (12)
C17—H17	0.9300	C47—H47	0.9300
C18—C19	1.366 (9)	C48—C49	1.347 (12)
C18—H18	0.9300	C48—H48	0.9300
C19—H19	0.9300	C49—C50	1.387 (11)
C20—C21	1.369 (10)	C49—H49	0.9300
C20—C25	1.381 (9)	C50—H50	0.9300
O1—Sn1—C8	95.4 (2)	C24—C23—H23	119.3
O1—Sn1—C20	108.9 (2)	C22—C23—H23	119.3
C8—Sn1—C20	111.4 (3)	C23—C24—C25	120.0 (8)
O1—Sn1—C14	107.4 (2)	C23—C24—H24	120.0
C8—Sn1—C14	114.5 (3)	C25—C24—H24	120.0
C20—Sn1—C14	116.8 (3)	C20—C25—C24	119.3 (7)
C45—Sn2—O4	106.3 (2)	C20—C25—H25	120.3
C45—Sn2—C33	125.0 (3)	C24—C25—H25	120.3
O4—Sn2—C33	100.3 (2)	O5—C26—O4	122.8 (7)
C45—Sn2—C39	112.4 (3)	O5—C26—C27	120.7 (8)
O4—Sn2—C39	95.2 (2)	O4—C26—C27	116.6 (8)
C33—Sn2—C39	112.0 (3)	C32—C27—C28	120.0 (9)
C1—O1—Sn1	113.8 (4)	C32—C27—C26	119.7 (8)
C3—O3—H3	109.5	C28—C27—C26	120.3 (9)
C26—O4—Sn2	113.3 (5)	O6—C28—C27	122.0 (10)
C28—O6—H6	109.5	O6—C28—C29	119.5 (10)
O2—C1—O1	122.2 (7)	C27—C28—C29	118.5 (11)
O2—C1—C2	120.8 (7)	C30—C29—C28	119.7 (15)
O1—C1—C2	116.9 (6)	C30—C29—H29	120.1
C7—C2—C3	119.5 (6)	C28—C29—H29	120.1
C7—C2—C1	120.2 (6)	C29—C30—C31	123.2 (16)
C3—C2—C1	120.3 (6)	C29—C30—H30	118.4
O3—C3—C2	123.2 (7)	C31—C30—H30	118.4
O3—C3—C4	117.6 (7)	C30—C31—C32	119.0 (12)
C2—C3—C4	119.2 (7)	C30—C31—Br2	122.5 (10)
C5—C4—C3	119.7 (7)	C32—C31—Br2	118.4 (9)
C5—C4—H4	120.1	C31—C32—C27	119.4 (9)
C3—C4—H4	120.1	C31—C32—H32	120.3
C6—C5—C4	120.3 (7)	C27—C32—H32	120.3
C6—C5—H5	119.9	C38—C33—C34	118.5 (7)
C4—C5—H5	119.9	C38—C33—Sn2	118.5 (6)
C5—C6—C7	120.3 (7)	C34—C33—Sn2	122.9 (6)
C5—C6—Br1	120.3 (6)	C33—C34—C35	121.2 (8)
C7—C6—Br1	119.4 (5)	C33—C34—H34	119.4
C6—C7—C2	120.9 (6)	C35—C34—H34	119.4
C6—C7—H7	119.6	C36—C35—C34	119.9 (10)

C2—C7—H7	119.6	C36—C35—H35	120.1
C9—C8—C13	115.9 (7)	C34—C35—H35	120.1
C9—C8—Sn1	124.1 (6)	C35—C36—C37	120.8 (10)
C13—C8—Sn1	120.1 (5)	C35—C36—H36	119.6
C8—C9—C10	122.7 (9)	C37—C36—H36	119.6
C8—C9—H9	118.6	C36—C37—C38	119.2 (10)
C10—C9—H9	118.6	C36—C37—H37	120.4
C11—C10—C9	119.0 (10)	C38—C37—H37	120.4
C11—C10—H10	120.5	C33—C38—C37	120.3 (9)
C9—C10—H10	120.5	C33—C38—H38	119.8
C12—C11—C10	121.0 (9)	C37—C38—H38	119.8
C12—C11—H11	119.5	C44—C39—C40	117.3 (7)
C10—C11—H11	119.5	C44—C39—Sn2	121.0 (6)
C11—C12—C13	120.0 (9)	C40—C39—Sn2	121.7 (6)
C11—C12—H12	120.0	C39—C40—C41	121.1 (8)
C13—C12—H12	120.0	C39—C40—H40	119.4
C12—C13—C8	121.4 (8)	C41—C40—H40	119.4
C12—C13—H13	119.3	C42—C41—C40	120.7 (9)
C8—C13—H13	119.3	C42—C41—H41	119.7
C19—C14—C15	118.6 (6)	C40—C41—H41	119.7
C19—C14—Sn1	121.8 (5)	C43—C42—C41	119.3 (9)
C15—C14—Sn1	119.6 (5)	C43—C42—H42	120.4
C14—C15—C16	119.0 (7)	C41—C42—H42	120.4
C14—C15—H15	120.5	C42—C43—C44	120.2 (8)
C16—C15—H15	120.5	C42—C43—H43	119.9
C17—C16—C15	120.4 (7)	C44—C43—H43	119.9
C17—C16—H16	119.8	C39—C44—C43	121.4 (8)
C15—C16—H16	119.8	C39—C44—H44	119.3
C18—C17—C16	120.0 (8)	C43—C44—H44	119.3
C18—C17—H17	120.0	C50—C45—C46	118.1 (7)
C16—C17—H17	120.0	C50—C45—Sn2	120.1 (6)
C17—C18—C19	121.3 (8)	C46—C45—Sn2	121.8 (6)
C17—C18—H18	119.4	C47—C46—C45	121.1 (9)
C19—C18—H18	119.4	C47—C46—H46	119.4
C18—C19—C14	120.8 (7)	C45—C46—H46	119.4
C18—C19—H19	119.6	C48—C47—C46	119.6 (10)
C14—C19—H19	119.6	C48—C47—H47	120.2
C21—C20—C25	117.9 (7)	C46—C47—H47	120.2
C21—C20—Sn1	121.6 (6)	C47—C48—C49	121.1 (10)
C25—C20—Sn1	120.4 (6)	C47—C48—H48	119.4
C20—C21—C22	122.2 (8)	C49—C48—H48	119.4
C20—C21—H21	118.9	C48—C49—C50	119.5 (9)
C22—C21—H21	118.9	C48—C49—H49	120.3
C23—C22—C21	119.0 (9)	C50—C49—H49	120.3
C23—C22—H22	120.5	C45—C50—C49	120.6 (8)
C21—C22—H22	120.5	C45—C50—H50	119.7
C24—C23—C22	121.4 (9)	C49—C50—H50	119.7

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.82	1.86	2.583 (8)	146
O6—H6···O5	0.82	1.86	2.583 (9)	147

Fig. 1


C49
C48
C5
Br1
C42
C41
C50
C6
C47
C4
C40
C43
C3
C7
C46
C45
C39
C44
C2
O3
Sn2
O4
C1
O1
O2
C32
C27
C31
C26
C9
C10
C21
C22
O5
C33
C8
Br2
C30
C29
C28
O6
C38
C34
Sn1
C11
C20
C23
C37
C14
C13
C12
C35
C19
C15
C36
C25
C24
C18
C16
C17