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Octabenzyldi-μ_2-methanolato-di-μ_3-oxido-bis(*p*-toluenesulfonato)tetratin(IV)

Shun-Li Li, Ting-Ting Han and Jin Yang*

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China
Correspondence e-mail: yangjinnenu@yahoo.com.cn

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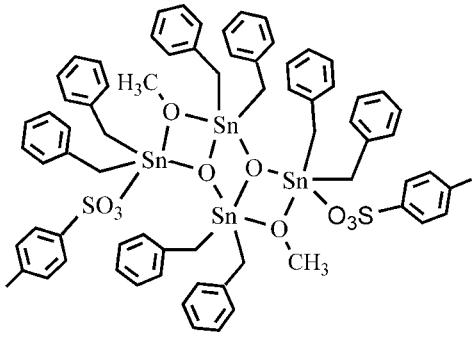
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.036; wR factor = 0.077; data-to-parameter ratio = 20.1.

The title compound, $[Sn_4(C_7H_7)_8(CH_3O)_2(C_7H_7O_3S)_2O_2]$, contains the well known structural unit of four organotin units linked by O-atom bridges into a ladder-type centrosymmetric tetramer. The Sn^{IV} atoms are coordinated in distorted SnC_2O_3 trigonal–bipyramidal geometries.

Related literature

For related literature, see: Chandrasekhar *et al.* (2003).



Experimental

Crystal data

$[Sn_4(C_7H_7)_8(CH_3O)_2(C_7H_7O_3S)_2O_2]$
M_r = 1640.21
Monoclinic, $P2_1/n$
a = 11.520 (5) Å
b = 11.302 (4) Å
c = 26.219 (11) Å
β = 99.409 (1)°
V = 3368 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 293 (2) K
0.43 × 0.15 × 0.13 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.747, T_{max} = 0.820
20431 measured reflections
7979 independent reflections
5980 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.077
S = 1.04
7979 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O1	2.176 (2)	Sn2—O2	2.047 (2)
Sn1—O2	2.008 (2)	Sn2—O2^{i}	2.148 (2)
Sn1—O5	2.260 (2)	Sn2—C7	2.146 (3)
Sn1—C21	2.134 (4)	Sn2—C14	2.142 (4)
Sn1—C28	2.140 (4)		

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2613).

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supplementary materials

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Octabenzyldi-μ_2-methanolato-di-μ_3-oxido-bis(*p*-toluenesulfonato)tetratin(IV)

S.-L. Li, T.-T. Han and J. Yang

Comment

Some organotin(IV) derivatives of sulfonates show antitumor activities (Chandrasekhar *et al.*, 2003). In this paper, we report the structure of a new organotin sulfonate, $[Sn_4(Bz)_8(L)_2(OCH_3)_2(O)_2]$, (I), where Bz = the benzyl group and *L* = *p*-toluenesulfonate.

Selected bond lengths for (I) are listed in Table 1. Both Sn(IV) atoms are five-coordinated in distorted trigonal–bipyramidal geometries. The *exo* tin atom (Sn1) is coordinated by two benzyl groups, one μ^3-O^{2-} anion, one μ^2-OCH_3^- anion and one *L* O atom. The *endo* tin atom (Sn2) is coordinated by two benzyl groups, two μ^3-O^{2-} anions, one μ^2-OCH_3^- anion and one *L* O atom. The four Sn(IV) atoms are connected by two μ^3-O^{2-} anions, generating the title Sn—O ladder structure. The *p*-toluenesulfonate anions and μ^2-OCH_3^- anion are attached on both sides of the ladder.

Experimental

A solution of *p*-toluenesulfonic aicd (100 mmol) in water (20 ml) was added to a mixture of Ag_2CO_3 (50 mmol) in water (20 ml). After stirring for several minutes until no CO_2 was given off, the white precipitate (AgL) was collected by removing the solvent *in vacuo*. Then a mixture of AgL (1.0 mmol) and Bz_2SnCl_2 (1.0 mmol) in CH_2Cl_2 (30 ml) were stirred continuously for 24 h at room temperature, the precipitate of AgCl was removed by filtration. Colourless blocks of (I) were obtained by evaporating the filtrate at room temperature.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.9and refined as riding atoms with C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip.

Figures

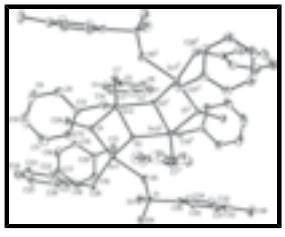


Fig. 1. View of (I) with displacement ellipsoids drawn at the 20% probability level and all H atoms omitted for clarity. Symmetry code: (i) $2-x$, $2-y$, $1-z$.

Octabenzyldi-μ$_2$-methanolato-di-μ$_3$-oxido-bis(*p*- toluenesulfonato)tetratin(IV)

Crystal data

$[Sn_4(C_7H_7)_8(CH_3O)_2(C_7H_7O_3S)_2O_2]$	F_{000} = 1640
M_r = 1640.21	D_x = 1.617 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2yn	Cell parameters from 7979 reflections
a = 11.520 (5) Å	θ = 1.6–28.4º
b = 11.302 (4) Å	μ = 1.59 mm^{-1}
c = 26.219 (11) Å	T = 293 (2) K
β = 99.409 (1)º	Block, colourless
V = 3368 (2) Å^3	0.43 × 0.15 × 0.13 mm
Z = 2	

Data collection

Bruker APEX CCD diffractometer	5980 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.033
T = 293(2) K	θ_{max} = 28.4º
ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −15→15
T_{min} = 0.747, T_{max} = 0.820	k = −15→11
20431 measured reflections	l = −24→34
7979 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H-atom parameters constrained
$wR(F^2)$ = 0.077	$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 0.8649P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
7979 reflections	$\Delta\rho_{max}$ = 0.74 e Å^{-3}
397 parameters	$\Delta\rho_{min}$ = −0.88 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6175 (4)	−0.1697 (5)	0.5096 (2)	0.0794 (15)
H1	0.5940	−0.1384	0.5391	0.095*
C2	0.5355 (4)	−0.1953 (5)	0.4674 (3)	0.0826 (17)
H2	0.4560	−0.1821	0.4679	0.099*
C3	0.5714 (4)	−0.2403 (4)	0.4247 (2)	0.0740 (15)
H3	0.5161	−0.2578	0.3957	0.089*
C4	0.6885 (4)	−0.2604 (3)	0.42368 (17)	0.0559 (11)
H4	0.7112	−0.2923	0.3941	0.067*
C5	0.7735 (3)	−0.2341 (3)	0.46587 (15)	0.0395 (9)
C6	0.7349 (4)	−0.1900 (4)	0.50868 (18)	0.0570 (11)
H6	0.7896	−0.1733	0.5380	0.068*
C7	0.9010 (3)	−0.2574 (3)	0.46511 (14)	0.0385 (9)
H7A	0.9066	−0.3123	0.4372	0.046*
H7B	0.9335	−0.2967	0.4972	0.046*
C8	1.2273 (4)	−0.2390 (4)	0.37217 (17)	0.0552 (11)
H8	1.2037	−0.3051	0.3889	0.066*
C9	1.2649 (4)	−0.2526 (5)	0.3254 (2)	0.0735 (15)
H9	1.2662	−0.3275	0.3108	0.088*
C10	1.3005 (4)	−0.1567 (6)	0.30022 (18)	0.0767 (15)
H10	1.3262	−0.1663	0.2686	0.092*
C11	1.2983 (4)	−0.0470 (5)	0.3216 (2)	0.0715 (14)
H11	1.3224	0.0186	0.3046	0.086*
C12	1.2600 (4)	−0.0331 (4)	0.36872 (17)	0.0559 (11)
H12	1.2588	0.0420	0.3830	0.067*
C13	1.2238 (3)	−0.1290 (3)	0.39479 (14)	0.0368 (8)
C14	1.1905 (3)	−0.1172 (3)	0.44700 (15)	0.0424 (9)
H14A	1.2291	−0.0467	0.4627	0.051*
H14B	1.2246	−0.1840	0.4674	0.051*
C15	0.5976 (3)	−0.0233 (3)	0.30526 (17)	0.0513 (11)
H15	0.6308	−0.0946	0.3180	0.062*
C16	0.5459 (4)	−0.0161 (4)	0.25441 (18)	0.0633 (13)
H16	0.5444	−0.0819	0.2330	0.076*
C17	0.4961 (4)	0.0893 (4)	0.23504 (18)	0.0659 (13)

H17	0.4617	0.0952	0.2005	0.079*
C18	0.4979 (4)	0.1853 (4)	0.26744 (17)	0.0598 (12)
H18	0.4635	0.2561	0.2548	0.072*
C19	0.5501 (3)	0.1771 (3)	0.31809 (16)	0.0498 (10)
H19	0.5508	0.2430	0.3394	0.060*
C20	0.6018 (3)	0.0730 (3)	0.33828 (15)	0.0421 (9)
C21	0.6640 (3)	0.0670 (3)	0.39339 (15)	0.0465 (10)
H21A	0.6591	−0.0129	0.4064	0.056*
H21B	0.6255	0.1195	0.4147	0.056*
C22	1.0230 (4)	0.1157 (4)	0.28211 (18)	0.0604 (12)
H22	1.0917	0.1228	0.3060	0.072*
C23	1.0255 (5)	0.0580 (4)	0.2367 (2)	0.0750 (14)
H23	1.0965	0.0274	0.2300	0.090*
C24	0.9264 (6)	0.0440 (4)	0.20063 (19)	0.0798 (16)
H24	0.9290	0.0030	0.1701	0.096*
C25	0.8232 (5)	0.0918 (4)	0.21050 (19)	0.0741 (15)
H25	0.7549	0.0839	0.1864	0.089*
C26	0.8202 (4)	0.1520 (4)	0.25627 (17)	0.0603 (12)
H26	0.7498	0.1850	0.2624	0.072*
C27	0.9203 (3)	0.1637 (3)	0.29309 (15)	0.0435 (9)
C28	0.9156 (4)	0.2233 (3)	0.34408 (15)	0.0543 (11)
H28A	0.8686	0.2946	0.3377	0.065*
H28B	0.9947	0.2470	0.3592	0.065*
C29	0.9053 (4)	−0.1259 (3)	0.33632 (14)	0.0498 (10)
H29A	0.8628	−0.0833	0.3075	0.075*
H29B	0.8621	−0.1956	0.3425	0.075*
H29C	0.9811	−0.1482	0.3288	0.075*
C30	0.8621 (3)	0.4827 (3)	0.53460 (15)	0.0453 (9)
H30	0.9356	0.4707	0.5251	0.054*
C31	0.8547 (4)	0.5357 (3)	0.58147 (16)	0.0509 (10)
H31	0.9231	0.5582	0.6033	0.061*
C32	0.7461 (4)	0.5556 (4)	0.59623 (18)	0.0595 (12)
C33	0.6469 (4)	0.5159 (4)	0.56382 (19)	0.0707 (14)
H33	0.5736	0.5252	0.5738	0.085*
C34	0.6540 (4)	0.4622 (4)	0.51658 (18)	0.0634 (12)
H34	0.5864	0.4366	0.4951	0.076*
C35	0.7634 (3)	0.4477 (3)	0.50208 (15)	0.0437 (9)
C36	0.7358 (5)	0.6198 (4)	0.6461 (2)	0.0920 (18)
H36A	0.8128	0.6414	0.6635	0.138*
H36B	0.6990	0.5688	0.6680	0.138*
H36C	0.6890	0.6898	0.6384	0.138*
O1	0.9200 (2)	−0.05216 (19)	0.38134 (8)	0.0369 (6)
O2	0.94751 (19)	0.06087 (18)	0.46365 (8)	0.0309 (5)
O3	0.6557 (3)	0.3742 (3)	0.41211 (12)	0.0726 (10)
O4	0.8481 (3)	0.4679 (2)	0.41599 (12)	0.0740 (9)
O5	0.8325 (2)	0.2759 (2)	0.44978 (10)	0.0483 (7)
Sn1	0.84442 (2)	0.116534 (19)	0.398869 (9)	0.03191 (7)
Sn2	1.009325 (19)	−0.106902 (18)	0.456013 (9)	0.02769 (7)
S1	0.77362 (9)	0.38944 (8)	0.43973 (4)	0.0467 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.056 (3)	0.089 (4)	0.100 (4)	−0.004 (3)	0.031 (3)	−0.015 (3)
C2	0.033 (3)	0.079 (4)	0.135 (6)	−0.006 (2)	0.012 (3)	0.005 (4)
C3	0.043 (3)	0.078 (3)	0.091 (4)	−0.013 (2)	−0.019 (3)	0.008 (3)
C4	0.054 (3)	0.056 (3)	0.053 (3)	−0.010 (2)	−0.004 (2)	0.000 (2)
C5	0.039 (2)	0.0277 (17)	0.050 (2)	−0.0040 (14)	0.0011 (18)	0.0042 (16)
C6	0.043 (2)	0.062 (3)	0.065 (3)	−0.009 (2)	0.007 (2)	−0.010 (2)
C7	0.042 (2)	0.0266 (17)	0.045 (2)	−0.0005 (14)	0.0030 (17)	0.0021 (15)
C8	0.054 (3)	0.051 (2)	0.063 (3)	−0.0043 (19)	0.018 (2)	−0.009 (2)
C9	0.061 (3)	0.089 (4)	0.075 (4)	−0.002 (3)	0.024 (3)	−0.038 (3)
C10	0.060 (3)	0.136 (5)	0.038 (3)	−0.012 (3)	0.020 (2)	−0.011 (3)
C11	0.063 (3)	0.094 (4)	0.060 (3)	−0.011 (3)	0.019 (3)	0.021 (3)
C12	0.061 (3)	0.054 (3)	0.056 (3)	−0.006 (2)	0.020 (2)	0.009 (2)
C13	0.0265 (17)	0.046 (2)	0.038 (2)	0.0017 (14)	0.0069 (15)	−0.0002 (16)
C14	0.0313 (19)	0.055 (2)	0.041 (2)	0.0035 (16)	0.0082 (16)	0.0006 (18)
C15	0.044 (2)	0.046 (2)	0.061 (3)	0.0000 (18)	0.001 (2)	−0.001 (2)
C16	0.059 (3)	0.066 (3)	0.062 (3)	−0.004 (2)	0.002 (2)	−0.022 (2)
C17	0.058 (3)	0.089 (4)	0.044 (3)	−0.008 (2)	−0.011 (2)	−0.002 (2)
C18	0.055 (3)	0.057 (3)	0.060 (3)	0.008 (2)	−0.011 (2)	0.010 (2)
C19	0.048 (2)	0.044 (2)	0.053 (3)	0.0027 (18)	−0.008 (2)	−0.0032 (19)
C20	0.034 (2)	0.043 (2)	0.046 (2)	−0.0010 (16)	−0.0008 (17)	−0.0018 (18)
C21	0.042 (2)	0.047 (2)	0.048 (2)	−0.0035 (17)	0.0024 (19)	0.0099 (19)
C22	0.058 (3)	0.072 (3)	0.051 (3)	−0.005 (2)	0.009 (2)	−0.001 (2)
C23	0.084 (4)	0.079 (3)	0.070 (4)	0.008 (3)	0.037 (3)	−0.005 (3)
C24	0.129 (5)	0.074 (3)	0.044 (3)	−0.019 (3)	0.038 (3)	−0.008 (2)
C25	0.082 (4)	0.099 (4)	0.039 (3)	−0.012 (3)	0.001 (3)	0.005 (3)
C26	0.060 (3)	0.071 (3)	0.050 (3)	0.001 (2)	0.011 (2)	0.016 (2)
C27	0.053 (2)	0.041 (2)	0.039 (2)	−0.0054 (18)	0.0135 (19)	0.0079 (17)
C28	0.082 (3)	0.040 (2)	0.043 (2)	−0.011 (2)	0.016 (2)	0.0018 (18)
C29	0.070 (3)	0.047 (2)	0.030 (2)	0.0069 (19)	−0.0003 (19)	−0.0088 (17)
C30	0.050 (2)	0.038 (2)	0.048 (3)	−0.0009 (17)	0.009 (2)	0.0003 (18)
C31	0.059 (3)	0.048 (2)	0.046 (3)	−0.0091 (19)	0.009 (2)	−0.0073 (19)
C32	0.069 (3)	0.054 (3)	0.056 (3)	0.000 (2)	0.014 (3)	−0.006 (2)
C33	0.058 (3)	0.089 (3)	0.070 (4)	0.011 (3)	0.025 (3)	−0.013 (3)
C34	0.045 (3)	0.079 (3)	0.065 (3)	0.009 (2)	0.007 (2)	−0.012 (3)
C35	0.051 (2)	0.037 (2)	0.045 (2)	0.0054 (17)	0.0098 (19)	−0.0037 (17)
C36	0.127 (5)	0.095 (4)	0.062 (3)	−0.003 (3)	0.041 (3)	−0.032 (3)
O1	0.0528 (15)	0.0330 (12)	0.0234 (13)	0.0078 (11)	0.0017 (11)	−0.0058 (10)
O2	0.0405 (13)	0.0277 (11)	0.0226 (12)	0.0075 (10)	−0.0002 (10)	−0.0002 (9)
O3	0.068 (2)	0.074 (2)	0.065 (2)	0.0164 (16)	−0.0195 (17)	−0.0156 (16)
O4	0.113 (3)	0.0529 (18)	0.064 (2)	−0.0100 (17)	0.038 (2)	0.0005 (15)
O5	0.0612 (17)	0.0426 (14)	0.0393 (15)	0.0127 (12)	0.0023 (13)	−0.0162 (12)
Sn1	0.03670 (14)	0.03096 (13)	0.02622 (13)	0.00300 (10)	−0.00032 (10)	0.00190 (10)
Sn2	0.03021 (12)	0.02620 (12)	0.02663 (12)	0.00233 (9)	0.00452 (9)	−0.00210 (9)
S1	0.0593 (6)	0.0383 (5)	0.0411 (6)	0.0080 (4)	0.0038 (5)	−0.0014 (4)

Geometric parameters (Å, °)

C1—C2	1.363 (7)	C22—H22	0.9300
C1—C6	1.376 (6)	C23—C24	1.368 (7)
C1—H1	0.9300	C23—H23	0.9300
C2—C3	1.354 (7)	C24—C25	1.367 (7)
C2—H2	0.9300	C24—H24	0.9300
C3—C4	1.372 (6)	C25—C26	1.385 (6)
C3—H3	0.9300	C25—H25	0.9300
C4—C5	1.384 (5)	C26—C27	1.384 (5)
C4—H4	0.9300	C26—H26	0.9300
C5—C6	1.367 (6)	C27—C28	1.506 (5)
C5—C7	1.495 (5)	C28—H28A	0.9700
C6—H6	0.9300	C28—H28B	0.9700
C7—H7A	0.9700	C29—O1	1.432 (4)
C7—H7B	0.9700	C29—H29A	0.9600
C8—C9	1.375 (6)	C29—H29B	0.9600
C8—C13	1.381 (5)	C29—H29C	0.9600
C8—H8	0.9300	C30—C35	1.364 (5)
C9—C10	1.366 (7)	C30—C31	1.382 (5)
C9—H9	0.9300	C30—H30	0.9300
C10—C11	1.363 (7)	C31—C32	1.387 (6)
C10—H10	0.9300	C31—H31	0.9300
C11—C12	1.387 (6)	C32—C33	1.383 (6)
C11—H11	0.9300	C32—C36	1.517 (6)
C12—C13	1.381 (5)	C33—C34	1.394 (6)
C12—H12	0.9300	C33—H33	0.9300
C13—C14	1.486 (5)	C34—C35	1.384 (6)
C14—H14A	0.9700	C34—H34	0.9300
C14—H14B	0.9700	C35—S1	1.784 (4)
C15—C16	1.371 (5)	C36—H36A	0.9600
C15—C20	1.387 (5)	C36—H36B	0.9600
C15—H15	0.9300	C36—H36C	0.9600
C16—C17	1.383 (6)	Sn1—O1	2.176 (2)
C16—H16	0.9300	Sn1—O2	2.008 (2)
C17—C18	1.376 (6)	Sn1—O5	2.260 (2)
C17—H17	0.9300	Sn1—C21	2.134 (4)
C18—C19	1.368 (5)	Sn1—C28	2.140 (4)
C18—H18	0.9300	Sn2—O2	2.047 (2)
C19—C20	1.384 (5)	Sn2—O2^{i}	2.148 (2)
C19—H19	0.9300	Sn2—O2^{i}	2.148 (2)
C20—C21	1.506 (5)	Sn2—C7	2.146 (3)
C21—H21A	0.9700	Sn2—C14	2.142 (4)
C21—H21B	0.9700	O3—S1	1.442 (3)
C22—C23	1.362 (6)	O4—S1	1.444 (3)
C22—C27	1.373 (6)	O5—S1	1.455 (2)
C2—C1—C6	120.2 (5)	C23—C24—H24	120.8

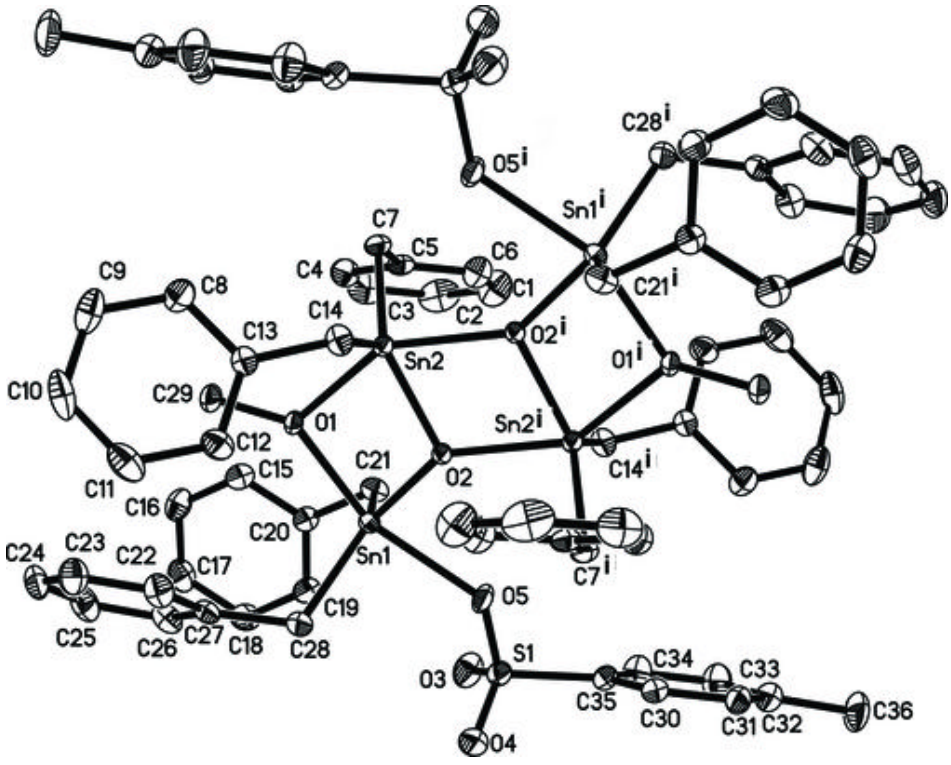
C2—C1—H1	119.9	C24—C25—C26	120.2 (5)
C6—C1—H1	119.9	C24—C25—H25	119.9
C3—C2—C1	119.0 (5)	C26—C25—H25	119.9
C3—C2—H2	120.5	C27—C26—C25	121.0 (5)
C1—C2—H2	120.5	C27—C26—H26	119.5
C2—C3—C4	120.9 (5)	C25—C26—H26	119.5
C2—C3—H3	119.6	C22—C27—C26	117.6 (4)
C4—C3—H3	119.6	C22—C27—C28	121.3 (4)
C3—C4—C5	121.2 (5)	C26—C27—C28	121.0 (4)
C3—C4—H4	119.4	C27—C28—Sn1	114.6 (2)
C5—C4—H4	119.4	C27—C28—H28A	108.6
C6—C5—C4	116.9 (4)	Sn1—C28—H28A	108.6
C6—C5—C7	121.8 (3)	C27—C28—H28B	108.6
C4—C5—C7	121.3 (4)	Sn1—C28—H28B	108.6
C5—C6—C1	121.8 (4)	H28A—C28—H28B	107.6
C5—C6—H6	119.1	O1—C29—H29A	109.5
C1—C6—H6	119.1	O1—C29—H29B	109.5
C5—C7—Sn2	116.9 (2)	H29A—C29—H29B	109.5
C5—C7—H7A	108.1	O1—C29—H29C	109.5
Sn2—C7—H7A	108.1	H29A—C29—H29C	109.5
C5—C7—H7B	108.1	H29B—C29—H29C	109.5
Sn2—C7—H7B	108.1	C35—C30—C31	121.0 (4)
H7A—C7—H7B	107.3	C35—C30—H30	119.5
C9—C8—C13	121.3 (4)	C31—C30—H30	119.5
C9—C8—H8	119.3	C30—C31—C32	120.5 (4)
C13—C8—H8	119.3	C30—C31—H31	119.7
C10—C9—C8	120.3 (4)	C32—C31—H31	119.7
C10—C9—H9	119.8	C33—C32—C31	117.9 (4)
C8—C9—H9	119.8	C33—C32—C36	120.7 (5)
C11—C10—C9	119.7 (4)	C31—C32—C36	121.3 (4)
C11—C10—H10	120.1	C32—C33—C34	121.7 (5)
C9—C10—H10	120.1	C32—C33—H33	119.2
C10—C11—C12	119.9 (4)	C34—C33—H33	119.2
C10—C11—H11	120.0	C35—C34—C33	119.0 (4)
C12—C11—H11	120.0	C35—C34—H34	120.5
C13—C12—C11	121.2 (4)	C33—C34—H34	120.5
C13—C12—H12	119.4	C30—C35—C34	119.8 (4)
C11—C12—H12	119.4	C30—C35—S1	120.5 (3)
C8—C13—C12	117.4 (4)	C34—C35—S1	119.7 (3)
C8—C13—C14	120.4 (3)	C32—C36—H36A	109.5
C12—C13—C14	122.0 (3)	C32—C36—H36B	109.5
C13—C14—Sn2	120.6 (2)	H36A—C36—H36B	109.5
C13—C14—H14A	107.2	C32—C36—H36C	109.5
Sn2—C14—H14A	107.2	H36A—C36—H36C	109.5
C13—C14—H14B	107.2	H36B—C36—H36C	109.5
Sn2—C14—H14B	107.2	C29—O1—Sn2	123.9 (2)
H14A—C14—H14B	106.8	C29—O1—Sn1	133.3 (2)
C16—C15—C20	121.7 (4)	Sn2—O1—Sn1	102.02 (9)
C16—C15—H15	119.1	Sn1—O2—Sn2	112.00 (10)

C20—C15—H15	119.1	Sn1—O2—Sn2^{i}	139.81 (11)
C15—C16—C17	119.8 (4)	Sn2—O2—Sn2^{i}	106.98 (9)
C15—C16—H16	120.1	S1—O5—Sn1	131.89 (15)
C17—C16—H16	120.1	O2—Sn1—C21	114.17 (12)
C18—C17—C16	119.3 (4)	O2—Sn1—C28	120.39 (14)
C18—C17—H17	120.4	C21—Sn1—C28	125.36 (16)
C16—C17—H17	120.4	O2—Sn1—O1	72.69 (8)
C19—C18—C17	120.4 (4)	C21—Sn1—O1	100.08 (13)
C19—C18—H18	119.8	C28—Sn1—O1	98.14 (13)
C17—C18—H18	119.8	O2—Sn1—O5	80.49 (9)
C18—C19—C20	121.4 (4)	C21—Sn1—O5	95.51 (13)
C18—C19—H19	119.3	C28—Sn1—O5	90.81 (13)
C20—C19—H19	119.3	O1—Sn1—O5	152.67 (9)
C19—C20—C15	117.4 (4)	O2—Sn2—C14	114.96 (12)
C19—C20—C21	120.9 (3)	O2—Sn2—C7	120.35 (12)
C15—C20—C21	121.7 (3)	C14—Sn2—C7	124.35 (13)
C20—C21—Sn1	111.0 (3)	O2—Sn2—O2^{i}	73.02 (9)
C20—C21—H21A	109.4	C14—Sn2—O2^{i}	92.74 (12)
Sn1—C21—H21A	109.4	C7—Sn2—O2^{i}	97.39 (11)
C20—C21—H21B	109.4	O2—Sn2—O1	72.54 (8)
Sn1—C21—H21B	109.4	C14—Sn2—O1	104.19 (12)
H21A—C21—H21B	108.0	C7—Sn2—O1	97.42 (11)
C23—C22—C27	121.0 (4)	O2^{i}—Sn2—O1	145.45 (8)
C23—C22—H22	119.5	O3—S1—O4	115.8 (2)
C27—C22—H22	119.5	O3—S1—O5	111.00 (16)
C22—C23—C24	121.6 (5)	O4—S1—O5	109.10 (19)
C22—C23—H23	119.2	O3—S1—C35	107.8 (2)
C24—C23—H23	119.2	O4—S1—C35	107.54 (18)
C25—C24—C23	118.5 (5)	O5—S1—C35	104.95 (16)
C25—C24—H24	120.8		
C6—C1—C2—C3	−0.3 (8)	Sn2—O2—Sn1—O5	178.26 (13)
C1—C2—C3—C4	0.2 (8)	Sn2^{i}—O2—Sn1—O5	13.22 (18)
C2—C3—C4—C5	−0.8 (7)	C20—C21—Sn1—O2	−160.3 (2)
C3—C4—C5—C6	1.5 (6)	C20—C21—Sn1—C28	22.7 (3)
C3—C4—C5—C7	179.2 (4)	C20—C21—Sn1—O1	−84.9 (3)
C4—C5—C6—C1	−1.7 (6)	C20—C21—Sn1—O5	117.6 (3)
C7—C5—C6—C1	−179.3 (4)	C27—C28—Sn1—O2	112.3 (3)
C2—C1—C6—C5	1.1 (7)	C27—C28—Sn1—C21	−70.9 (4)
C6—C5—C7—Sn2	−77.6 (4)	C27—C28—Sn1—O1	37.7 (3)
C4—C5—C7—Sn2	104.8 (3)	C27—C28—Sn1—O5	−168.2 (3)
C13—C8—C9—C10	0.3 (7)	C29—O1—Sn1—O2	176.6 (3)
C8—C9—C10—C11	−0.2 (8)	Sn2—O1—Sn1—O2	6.36 (9)
C9—C10—C11—C12	0.1 (7)	C29—O1—Sn1—C21	64.2 (3)
C10—C11—C12—C13	0.0 (7)	Sn2—O1—Sn1—C21	−105.98 (13)
C9—C8—C13—C12	−0.3 (6)	C29—O1—Sn1—C28	−64.0 (3)
C9—C8—C13—C14	−175.8 (4)	Sn2—O1—Sn1—C28	125.75 (14)
C11—C12—C13—C8	0.1 (6)	C29—O1—Sn1—O5	−171.9 (3)

C11—C12—C13—C14	175.6 (4)	Sn2—O1—Sn1—O5	17.8 (3)
C8—C13—C14—Sn2	−85.0 (4)	S1—O5—Sn1—O2	177.3 (2)
C12—C13—C14—Sn2	99.6 (4)	S1—O5—Sn1—C21	−69.1 (2)
C20—C15—C16—C17	−0.1 (7)	S1—O5—Sn1—C28	56.6 (3)
C15—C16—C17—C18	−0.8 (7)	S1—O5—Sn1—O1	166.20 (17)
C16—C17—C18—C19	1.0 (7)	Sn1—O2—Sn2—C14	105.02 (14)
C17—C18—C19—C20	−0.3 (7)	$Sn2^{i}$—O2—Sn2—C14	−85.01 (15)
C18—C19—C20—C15	−0.6 (6)	Sn1—O2—Sn2—C7	−81.28 (16)
C18—C19—C20—C21	177.0 (4)	$Sn2^{i}$—O2—Sn2—C7	88.68 (14)
C16—C15—C20—C19	0.8 (6)	Sn1—O2—Sn2—$O2^{i}$	−169.97 (18)
C16—C15—C20—C21	−176.8 (4)	$Sn2^{i}$—O2—Sn2—$O2^{i}$	0.0
C19—C20—C21—Sn1	−88.0 (4)	Sn1—O2—Sn2—O1	7.15 (10)
C15—C20—C21—Sn1	89.5 (4)	$Sn2^{i}$—O2—Sn2—O1	177.12 (13)
C27—C22—C23—C24	−0.9 (7)	C13—C14—Sn2—O2	−97.7 (3)
C22—C23—C24—C25	1.4 (8)	C13—C14—Sn2—C7	88.9 (3)
C23—C24—C25—C26	−0.5 (8)	C13—C14—Sn2—$O2^{i}$	−170.2 (3)
C24—C25—C26—C27	−0.9 (7)	C13—C14—Sn2—O1	−20.6 (3)
C23—C22—C27—C26	−0.4 (6)	C5—C7—Sn2—O2	12.6 (3)
C23—C22—C27—C28	177.5 (4)	C5—C7—Sn2—C14	−174.4 (3)
C25—C26—C27—C22	1.3 (6)	C5—C7—Sn2—$O2^{i}$	87.2 (3)
C25—C26—C27—C28	−176.6 (4)	C5—C7—Sn2—O1	−61.5 (3)
C22—C27—C28—Sn1	−100.3 (4)	C29—O1—Sn2—O2	−177.7 (3)
C26—C27—C28—Sn1	77.5 (4)	Sn1—O1—Sn2—O2	−6.25 (9)
C35—C30—C31—C32	−0.7 (6)	C29—O1—Sn2—C14	70.2 (3)
C30—C31—C32—C33	3.0 (6)	Sn1—O1—Sn2—C14	−118.38 (13)
C30—C31—C32—C36	−176.5 (4)	C29—O1—Sn2—C7	−58.1 (3)
C31—C32—C33—C34	−2.9 (7)	Sn1—O1—Sn2—C7	113.31 (13)
C36—C32—C33—C34	176.6 (5)	C29—O1—Sn2—$O2^{i}$	−172.8 (2)
C32—C33—C34—C35	0.5 (7)	Sn1—O1—Sn2—$O2^{i}$	−1.4 (2)
C31—C30—C35—C34	−1.8 (6)	Sn1—O5—S1—O3	45.4 (3)
C31—C30—C35—S1	175.4 (3)	Sn1—O5—S1—O4	−83.3 (2)
C33—C34—C35—C30	1.9 (6)	Sn1—O5—S1—C35	161.7 (2)
C33—C34—C35—S1	−175.3 (3)	C30—C35—S1—O3	−173.1 (3)
Sn2—O2—Sn1—C21	86.45 (16)	C34—C35—S1—O3	4.1 (4)
$Sn2^{i}$—O2—Sn1—C21	−78.6 (2)	C30—C35—S1—O4	−47.5 (4)
Sn2—O2—Sn1—C28	−96.43 (16)	C34—C35—S1—O4	129.6 (4)
$Sn2^{i}$—O2—Sn1—C28	98.5 (2)	C30—C35—S1—O5	68.5 (3)
Sn2—O2—Sn1—O1	−7.05 (10)	C34—C35—S1—O5	−114.3 (3)
$Sn2^{i}$—O2—Sn1—O1	−172.1 (2)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

Fig. 1


C28i
O5i
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C31
C32
C36
O4