

Di- μ_3 -oxo-bis(μ_2 -2,3,4,5-tetrafluorobenzoato- κ^2 O:O')bis(2,3,4,5-tetrafluorobenzoato- κ O)tetrakis[dimethyltin(IV)]

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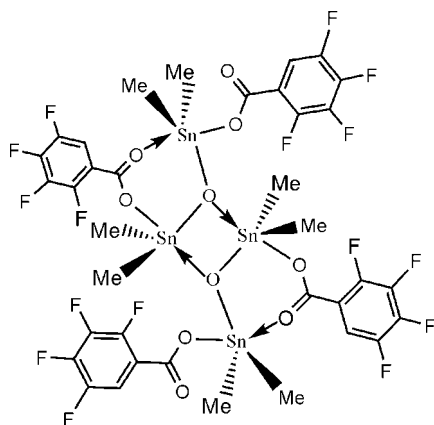
Received 24 June 2007; accepted 25 June 2007

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.015$ Å; R factor = 0.052; wR factor = 0.159; data-to-parameter ratio = 13.7.

The title compound, $[\text{Sn}_4(\text{CH}_3)_8(\text{C}_7\text{HF}_4\text{O}_2)_4\text{O}_2]$, was obtained from the reaction of the ligand 2,3,4,5-tetrafluorobenzoic acid and dimethyltin(IV) oxide. The Sn atom is five-coordinate and displays trigonal-bipyramidal geometry. The molecule is centrosymmetric about the $\text{Me}_4\text{Sn}_2\text{O}_2$ core and molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ intermolecular interactions.

Related literature

Related examples have wide-ranging applications (Davies, 1997), and a large number of organotin carboxylate complexes have been reported (Gielen, 2002), though only a few fluorinated ligands have been used in organotin complexes (Gielen *et al.*, 1995; Sun *et al.*, 2007). For related literature, see: Bondi (1964).



Experimental

Crystal data

$[\text{Sn}_4(\text{CH}_3)_8(\text{C}_7\text{HF}_4\text{O}_2)_4\text{O}_2]$
 $M_r = 1399.34$
Triclinic, $P\bar{1}$
 $a = 7.6590$ (9) Å
 $b = 11.1358$ (13) Å
 $c = 14.6746$ (17) Å
 $\alpha = 107.634$ (15)°
 $\beta = 100.296$ (16)°

$\gamma = 100.185$ (16)°
 $V = 1137.4$ (3) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 2.29$ mm⁻¹
 $T = 298$ (2) K
 $0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
 $T_{\min} = 0.454$, $T_{\max} = 0.502$
(expected range = 0.406–0.449)

5695 measured reflections
3908 independent reflections
2795 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.159$
 $S = 1.01$
3908 reflections
286 parameters

49 restraints
H-atom parameters constrained
 $\Delta\rho_{\max} = 2.05$ e Å⁻³
 $\Delta\rho_{\min} = -2.31$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Sn1—O3	2.053 (5)	Sn2—O2	2.202 (6)
Sn1—O3 ⁱ	2.140 (6)	Sn2—O3	2.022 (5)
Sn1—O4	2.270 (5)	Sn2—O5	2.295 (7)
C10—Sn1—C11	142.7 (4)	Sn2—O3—Sn1 ⁱ	124.2 (2)
C8—Sn2—C9	146.4 (5)	Sn1—O3—Sn1 ⁱ	103.4 (2)
Sn2—O3—Sn1	132.2 (3)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C3—H3 ⁱⁱ ⋯O1 ⁱⁱ	0.93	2.49	3.375 (12)	160
C8—H8C ⁱⁱⁱ ⋯F3 ⁱⁱⁱ	0.96	2.44	3.347 (14)	159
C11—H11B ^{iv} ⋯F6 ^{iv}	0.96	2.61	3.441 (11)	145

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (20271025) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2018).

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supplementary materials

Acta Cryst. (2007). E63, m2035-m2036 [doi:10.1107/S1600536807031030]

Di- μ_3 -oxo-bis(μ_2 -2,3,4,5-tetrafluorobenzoato- $\kappa^2 O:O'$)bis(2,3,4,5-tetrafluorobenzoato- κO)tetrakis[dimethyltin(IV)]

L.-L. Qiu, J.-S. Sun, J.-K. Li and R.-F. Zhang

Comment

Organotin(IV) carboxylates form an important class of compounds and have received much interest in recent years, not only due to their intrinsic interest but owing to their varied applications. Some examples have found wide use as catalysts and stabilizers, and certain derivatives are used as biocides, as antifouling agents and as wood preservatives (Davies, 1997). In order to explore the impact of the structure on the properties of the complexes, as well as to analyze structure-activity relationships, a large number of organotin carboxylate complexes have been prepared and studied (Gielen, 2002). However, only few fluorinated ligands have been used in organotin complexes (Gielen *et al.*, 1995). The 2,3,4,5-tetrafluorobenzoic acid is one of the most common ligands of this type, and herein, we report the structure of the title complex, $\{[(F_4C_6HCO_2)(CH_3)_2Sn]_2O\}_2$.

The molecule structure and the unit cell of the title complex is shown in Figs 1 and 2, respectively. The structure is centrosymmetric about a $Me_4Sn_2O_2$ core. Two oxygen atoms of this unit are tridentate as they link three Sn centres, two *endo*-cyclic and one *exo*-cyclic. Pairs of Sn atoms are bridged by bidentate carboxylate ligands and the external Sn atoms have their coordination geometry completed by a monodentate carboxylate ligand. The tin atom geometries are similar and are based on a five-coordinated trigonal bipyramidal arrangement. The Sn—O bond lengths are Sn(1)—O(4) 2.275 (6) Å, Sn(1)—O(5) 2.293 (6) Å and Sn(2)—O(2) 2.200 (5) Å, which are close to the covalent radii of Sn and O (2.13 Å) (Bondi, 1964), showing the strong coordination interaction. The axis angles for the geometry are C(10)—Sn(1)—C(11) 142.9 (3)° and C(9)—Sn(2)—C(8) 146.5 (4)°, showing a large deviation.

Experimental

All reagents and solvents were used as obtained without further purification. The reaction was carried out under N_2 atmosphere. The 2,3,4,5-tetrafluorobenzoic acid (0.239 g, 1 mmol) and dimethyltin oxide (0.165 g, 1 mmol) were added to a solution of dry benzene (30 ml) in a Schlenk flask and stirred under reflux conditions 12 h at 353 K; then dimethyltin oxide (0.220 g, 1 mmol) was added. After cooling to the room temperature, the solution was filtered. The solvent was removed from the filtrate under vacuum, and the solid residue was recrystallized from diethyl ether; colorless crystals suitable for an X-ray diffraction study were obtained. Yield, 81%. m.p. 134–136 °C. Analysis, calculated for $C_{36}H_{28}O_{10}F_{16}Sn_4$: C 30.90, H 2.02; found: C 30.72, H 2.26. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II. The number of CCDC: 631570.

Refinement

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with aromatic and methyl C—H distances of 0.93 Å and 0.96 Å, respectively. The $U_{iso}(H)$ values were set at $1.2U_{eq}(C)$ for the aromatic and $1.5U_{eq}(C)$ for the methyl H atoms.

Figures

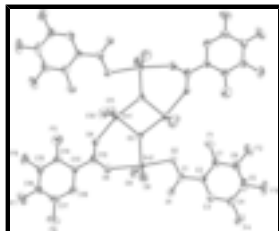


Fig. 1. The molecular structure of (I) with atom numbering and with 30% probability displacement ellipsoids for non-H atoms.



Fig. 2. The unit cell of the molecular structure.

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Crystal data

[Sn₄(CH₃)₈(C₇HF₄O₂)₄O₂]

$M_r = 1399.34$

Triclinic, *PT*

Hall symbol: -P 1

$a = 7.6590$ (9) Å

$b = 11.1358$ (13) Å

$c = 14.6746$ (17) Å

$\alpha = 107.634$ (15)°

$\beta = 100.296$ (16)°

$\gamma = 100.185$ (16)°

$V = 1137.4$ (3) Å³

$Z = 1$

$F_{000} = 668$

$D_x = 2.043$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2453 reflections

$\theta = 2.8$ – 26.7°

$\mu = 2.29$ mm⁻¹

$T = 298$ (2) K

Block, colourless

$0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2004)

$T_{\min} = 0.454$, $T_{\max} = 0.502$

5695 measured reflections

3908 independent reflections

2795 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 2.0^\circ$

$h = -9 \rightarrow 7$

$k = -12 \rightarrow 13$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.052$$

$$wR(F^2) = 0.159$$

$$S = 1.01$$

3908 reflections

286 parameters

49 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0982P)^2]$$

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

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

$$\Delta\rho_{\max} = 2.05 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -2.31 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.91008 (8)	0.35427 (5)	0.49974 (4)	0.0401 (2)
Sn2	0.95074 (8)	0.38429 (6)	0.25786 (4)	0.0410 (2)
O1	0.9747 (10)	0.5044 (6)	0.1239 (4)	0.0672 (17)
O2	1.0227 (8)	0.5943 (6)	0.2837 (4)	0.0514 (15)
O3	0.9703 (8)	0.4488 (5)	0.4047 (4)	0.0435 (13)
O4	0.7690 (7)	0.1671 (5)	0.3715 (4)	0.0401 (2)
O5	0.9078 (10)	0.1726 (6)	0.2520 (5)	0.0646 (17)
F1	1.1574 (10)	0.8538 (6)	0.3612 (4)	0.083 (2)
F2	1.2903 (10)	1.0721 (6)	0.3325 (5)	0.093 (2)
F3	1.3077 (12)	1.0710 (7)	0.1490 (7)	0.116 (3)
F4	1.1862 (14)	0.8501 (8)	-0.0062 (6)	0.122 (3)
F5	0.6430 (12)	-0.0636 (8)	0.3815 (6)	0.113 (3)
F6	0.5008 (9)	-0.3119 (6)	0.2845 (5)	0.0814 (19)
F7	0.5109 (11)	-0.4186 (6)	0.0952 (6)	0.104 (3)
F8	0.6718 (10)	-0.2728 (7)	0.0024 (4)	0.097 (2)
C1	1.0236 (16)	0.6013 (10)	0.1976 (7)	0.0672 (17)
C2	1.0997 (12)	0.7292 (9)	0.1896 (6)	0.045 (2)
C3	1.1112 (15)	0.7308 (10)	0.0985 (8)	0.064 (3)
H3	1.0701	0.6538	0.0446	0.076*
C4	1.1825 (17)	0.8445 (12)	0.0850 (9)	0.072 (3)
C5	1.2464 (15)	0.9593 (11)	0.1635 (11)	0.077 (4)

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C6	1.2274 (14)	0.9605 (10)	0.2543 (8)	0.063 (3)
C7	1.1614 (13)	0.8462 (9)	0.2689 (7)	0.055 (2)
C8	1.2081 (14)	0.3590 (10)	0.2339 (8)	0.066 (3)
H8A	1.3010	0.4031	0.2944	0.099*
H8B	1.2354	0.3944	0.1845	0.099*
H8C	1.2048	0.2680	0.2119	0.099*
C9	0.6708 (14)	0.3455 (12)	0.1955 (8)	0.087 (4)
H9A	0.6119	0.3854	0.2450	0.130*
H9B	0.6196	0.2532	0.1699	0.130*
H9C	0.6521	0.3799	0.1430	0.130*
C10	1.1306 (15)	0.2745 (12)	0.5321 (8)	0.074 (3)
H10A	1.2302	0.3099	0.5088	0.110*
H10B	1.0937	0.1818	0.5000	0.110*
H10C	1.1692	0.2951	0.6021	0.110*
C11	0.6381 (12)	0.3513 (10)	0.5138 (7)	0.056 (2)
H11A	0.5921	0.4102	0.4855	0.085*
H11B	0.6375	0.3774	0.5823	0.085*
H11C	0.5618	0.2649	0.4798	0.085*
C12	0.8051 (12)	0.1130 (9)	0.2903 (7)	0.049 (2)
C13	0.7312 (11)	-0.0276 (8)	0.2416 (6)	0.041 (2)
C14	0.6521 (12)	-0.1085 (10)	0.2872 (6)	0.050 (2)
C15	0.5775 (13)	-0.2391 (9)	0.2366 (8)	0.056 (3)
C16	0.5824 (14)	-0.2943 (10)	0.1427 (7)	0.060 (3)
C17	0.6605 (15)	-0.2171 (11)	0.0972 (7)	0.067 (3)
C18	0.7351 (13)	-0.0850 (10)	0.1422 (7)	0.052 (2)
H18	0.7863	-0.0356	0.1083	0.063*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0434 (4)	0.0388 (4)	0.0411 (3)	0.0045 (3)	0.0175 (3)	0.0174 (3)
Sn2	0.0461 (4)	0.0405 (4)	0.0351 (3)	0.0027 (3)	0.0139 (3)	0.0134 (3)
O1	0.093 (4)	0.047 (3)	0.052 (3)	-0.005 (3)	0.018 (3)	0.016 (3)
O2	0.070 (4)	0.049 (3)	0.040 (3)	0.009 (3)	0.021 (3)	0.020 (3)
O3	0.053 (3)	0.041 (3)	0.038 (3)	0.003 (2)	0.020 (2)	0.016 (2)
O4	0.0434 (4)	0.0388 (4)	0.0411 (3)	0.0045 (3)	0.0175 (3)	0.0174 (3)
O5	0.086 (4)	0.049 (3)	0.056 (3)	0.003 (3)	0.029 (3)	0.016 (3)
F1	0.125 (6)	0.064 (4)	0.048 (3)	0.008 (4)	0.027 (3)	0.008 (3)
F2	0.103 (5)	0.044 (4)	0.110 (6)	0.001 (3)	0.025 (4)	0.005 (4)
F3	0.144 (7)	0.058 (5)	0.175 (8)	0.015 (4)	0.074 (6)	0.066 (5)
F4	0.214 (10)	0.087 (6)	0.094 (5)	0.029 (6)	0.080 (6)	0.054 (5)
F5	0.148 (8)	0.101 (6)	0.087 (5)	0.009 (5)	0.046 (5)	0.030 (5)
F6	0.085 (4)	0.063 (4)	0.096 (5)	-0.005 (3)	0.022 (4)	0.040 (4)
F7	0.115 (6)	0.045 (4)	0.109 (6)	-0.008 (4)	0.000 (4)	-0.002 (4)
F8	0.109 (6)	0.106 (6)	0.053 (4)	0.018 (4)	0.021 (4)	-0.003 (4)
C1	0.093 (4)	0.047 (3)	0.052 (3)	-0.005 (3)	0.018 (3)	0.016 (3)
C2	0.046 (5)	0.043 (5)	0.044 (5)	0.007 (4)	0.010 (4)	0.016 (4)
C3	0.086 (8)	0.046 (6)	0.059 (6)	0.009 (5)	0.024 (6)	0.018 (5)

C4	0.094 (9)	0.064 (8)	0.082 (8)	0.019 (6)	0.047 (7)	0.046 (7)
C5	0.071 (7)	0.051 (7)	0.135 (11)	0.023 (6)	0.042 (8)	0.055 (8)
C6	0.066 (7)	0.045 (6)	0.081 (7)	0.014 (5)	0.032 (6)	0.018 (6)
C7	0.056 (6)	0.048 (6)	0.065 (6)	0.014 (5)	0.019 (5)	0.022 (5)
C8	0.068 (7)	0.052 (6)	0.090 (8)	0.016 (5)	0.044 (6)	0.026 (6)
C9	0.065 (7)	0.096 (10)	0.082 (8)	-0.013 (7)	-0.002 (6)	0.037 (7)
C10	0.077 (7)	0.095 (9)	0.080 (7)	0.055 (7)	0.035 (6)	0.046 (7)
C11	0.041 (5)	0.066 (7)	0.057 (6)	0.006 (5)	0.015 (4)	0.016 (5)
C12	0.043 (5)	0.040 (5)	0.073 (6)	0.014 (4)	0.028 (5)	0.025 (5)
C13	0.039 (5)	0.036 (5)	0.046 (5)	0.004 (4)	0.010 (4)	0.016 (4)
C14	0.048 (5)	0.060 (6)	0.040 (4)	0.010 (4)	0.007 (4)	0.020 (4)
C15	0.047 (6)	0.044 (6)	0.074 (7)	-0.001 (4)	0.009 (5)	0.025 (5)
C16	0.066 (7)	0.038 (6)	0.053 (6)	0.005 (5)	-0.006 (5)	0.001 (5)
C17	0.073 (7)	0.073 (8)	0.036 (5)	0.008 (6)	0.008 (5)	0.001 (5)
C18	0.056 (6)	0.060 (6)	0.043 (5)	0.012 (5)	0.011 (4)	0.023 (5)

Geometric parameters (Å, °)

Sn1—O3	2.053 (5)	C3—C4	1.373 (14)
Sn1—O3 ⁱ	2.140 (6)	C3—H3	0.9300
Sn1—O4	2.270 (5)	C4—C5	1.374 (17)
Sn1—C10	2.090 (9)	C5—C6	1.362 (15)
Sn1—C11	2.125 (9)	C6—C7	1.378 (14)
Sn2—O2	2.202 (6)	C8—H8A	0.9600
Sn2—O3	2.022 (5)	C8—H8B	0.9600
Sn2—O5	2.295 (7)	C8—H8C	0.9600
Sn2—C8	2.115 (9)	C9—H9A	0.9600
Sn2—C9	2.086 (10)	C9—H9B	0.9600
O1—C1	1.216 (11)	C9—H9C	0.9600
O2—C1	1.291 (11)	C10—H10A	0.9600
O3—Sn1 ⁱ	2.140 (6)	C10—H10B	0.9600
O4—C12	1.265 (10)	C10—H10C	0.9600
O5—C12	1.255 (10)	C11—H11A	0.9600
F1—C7	1.337 (11)	C11—H11B	0.9600
F2—C6	1.350 (12)	C11—H11C	0.9600
F3—C5	1.342 (11)	C12—C13	1.466 (12)
F4—C4	1.363 (12)	C13—C14	1.394 (12)
F5—C14	1.341 (11)	C13—C18	1.412 (12)
F6—C15	1.348 (11)	C14—C15	1.376 (13)
F7—C16	1.309 (12)	C15—C16	1.339 (14)
F8—C17	1.366 (11)	C16—C17	1.361 (15)
C1—C2	1.488 (13)	C17—C18	1.380 (14)
C2—C3	1.359 (12)	C18—H18	0.9300
C2—C7	1.394 (13)		
O3—Sn1—C10	106.3 (3)	F1—C7—C6	117.1 (9)
O3—Sn1—C11	110.2 (3)	F1—C7—C2	122.5 (8)
C10—Sn1—C11	142.7 (4)	C6—C7—C2	120.4 (9)
O3—Sn1—O3 ⁱ	76.6 (2)	Sn2—C8—H8A	109.5

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C10—Sn1—O3 ⁱ	98.8 (4)	Sn2—C8—H8B	109.5
C11—Sn1—O3 ⁱ	96.5 (3)	H8A—C8—H8B	109.5
O3—Sn1—O4	91.1 (2)	Sn2—C8—H8C	109.5
C10—Sn1—O4	89.5 (4)	H8A—C8—H8C	109.5
C11—Sn1—O4	82.8 (3)	H8B—C8—H8C	109.5
O3 ⁱ —Sn1—O4	166.7 (2)	Sn2—C9—H9A	109.5
O3—Sn1—Sn1 ⁱ	39.25 (15)	Sn2—C9—H9B	109.5
C10—Sn1—Sn1 ⁱ	106.0 (3)	H9A—C9—H9B	109.5
C11—Sn1—Sn1 ⁱ	106.8 (3)	Sn2—C9—H9C	109.5
O3 ⁱ —Sn1—Sn1 ⁱ	37.36 (13)	H9A—C9—H9C	109.5
O4—Sn1—Sn1 ⁱ	130.19 (13)	H9B—C9—H9C	109.5
O3—Sn2—C9	103.5 (4)	Sn1—C10—H10A	109.5
O3—Sn2—C8	109.1 (4)	Sn1—C10—H10B	109.5
C8—Sn2—C9	146.4 (5)	H10A—C10—H10B	109.5
O3—Sn2—O2	82.0 (2)	Sn1—C10—H10C	109.5
C9—Sn2—O2	98.5 (4)	H10A—C10—H10C	109.5
C8—Sn2—O2	93.8 (3)	H10B—C10—H10C	109.5
O3—Sn2—O5	91.7 (2)	Sn1—C11—H11A	109.5
C9—Sn2—O5	88.4 (4)	Sn1—C11—H11B	109.5
C8—Sn2—O5	82.9 (3)	H11A—C11—H11B	109.5
O2—Sn2—O5	171.6 (2)	Sn1—C11—H11C	109.5
C1—O2—Sn2	104.4 (6)	H11A—C11—H11C	109.5
Sn2—O3—Sn1	132.2 (3)	H11B—C11—H11C	109.5
Sn2—O3—Sn1 ⁱ	124.2 (2)	O5—C12—O4	123.3 (8)
Sn1—O3—Sn1 ⁱ	103.4 (2)	O5—C12—C13	118.5 (8)
C12—O4—Sn1	132.8 (5)	O4—C12—C13	118.1 (7)
C12—O5—Sn2	129.0 (6)	C14—C13—C18	117.6 (8)
O1—C1—O2	121.3 (9)	C14—C13—C12	123.6 (8)
O1—C1—C2	119.4 (9)	C18—C13—C12	118.8 (8)
O2—C1—C2	119.1 (9)	F5—C14—C15	116.6 (9)
C3—C2—C7	118.2 (8)	F5—C14—C13	122.2 (9)
C3—C2—C1	117.3 (8)	C15—C14—C13	121.2 (8)
C7—C2—C1	124.4 (8)	C16—C15—F6	120.2 (9)
C2—C3—C4	121.0 (10)	C16—C15—C14	121.5 (9)
C2—C3—H3	119.5	F6—C15—C14	118.4 (9)
C4—C3—H3	119.5	F7—C16—C15	121.0 (11)
F4—C4—C3	122.2 (11)	F7—C16—C17	120.8 (10)
F4—C4—C5	117.1 (10)	C15—C16—C17	118.2 (9)
C3—C4—C5	120.7 (10)	C16—C17—F8	118.8 (10)
F3—C5—C6	120.3 (12)	C16—C17—C18	123.8 (9)
F3—C5—C4	120.3 (12)	F8—C17—C18	117.4 (10)
C6—C5—C4	118.9 (9)	C17—C18—C13	117.8 (9)
F2—C6—C5	119.8 (10)	C17—C18—H18	121.1
F2—C6—C7	119.4 (10)	C13—C18—H18	121.1
C5—C6—C7	120.4 (10)		

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

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>
C3—H3···O1 ⁱⁱ	0.93	2.49	3.375 (12)	160
C8—H8C···F3 ⁱⁱⁱ	0.96	2.44	3.347 (14)	159
C11—H11B···F6 ^{iv}	0.96	2.61	3.441 (11)	145

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

Fig. 2

