Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dimethyl(1,10-phenanthroline)-bis(2,3,4,5-tetrafluorobenzoato)tin(IV)

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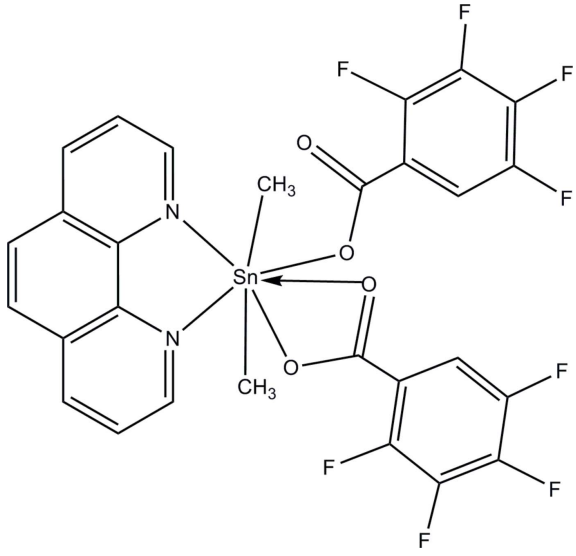
Received 26 September 2007; accepted 2 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.016 Å; R factor = 0.081; wR factor = 0.222; data-to-parameter ratio = 11.6.

The title compound, $[Sn(CH_3)_2(C_7HF_4O_2)_2(C_{12}H_8N_2)]$, was synthesized by the reaction of dimethyltin(IV) dichloride and disodium 2,3,4,5-tetrafluorobenzoate in the presence of 1,10-phenanthroline. In the complex, the Sn^{IV} ion is coordinated by three O atoms of two tetrafluorobenzoate ligands, two N atoms of a 1,10-phenanthroline ligand and two methyl groups in a distorted pentagonal–bipyramidal coordination. The axial positions are occupied by the methyl groups. In the crystal structure, C—H···F and C—H···O hydrogen bonds link the molecules into cyclic centrosymmetric dimers.

Related literature

For applications of organotin carboxylate complexes, see: Narula *et al.* (1988). For related structures, see: Gielen (2002); Li *et al.* (2005). For van der Waals radii and covalent radii data, see: Casas *et al.* (1997); Ma *et al.* (2005).



Experimental

Crystal data

$[Sn(CH_3)_2(C_7HF_4O_2)_2(C_{12}H_8N_2)]$
M_r = 715.12
Triclinic, $P\overline{1}$
a = 7.265 (4) Å
b = 10.174 (6) Å
c = 18.957 (11) Å
α = 90.519 (10)°
β = 90.205 (9)°
γ = 110.247 (8)°
V = 1314.5 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 298 (2) K
0.18 × 0.13 × 0.09 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.831, T_{max} = 0.910
6410 measured reflections
4483 independent reflections
3007 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.222
S = 1.01
4483 reflections
388 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −2.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C27	2.072 (13)	Sn1—N2	2.389 (8)
Sn1—C28	2.092 (13)	Sn1—N1	2.472 (8)
Sn1—O3	2.146 (7)	Sn1—O1	2.554 (8)
Sn1—O2	2.360 (7)		
C27—Sn1—C28	173.1 (4)	C28—Sn1—N1	87.6 (4)
C27—Sn1—O3	95.4 (4)	O3—Sn1—N1	153.2 (3)
C28—Sn1—O3	91.1 (4)	O2—Sn1—N1	129.2 (3)
C27—Sn1—O2	88.2 (4)	N2—Sn1—N1	67.6 (3)
C28—Sn1—O2	90.9 (4)	C27—Sn1—O1	85.9 (4)
O3—Sn1—O2	77.6 (3)	C28—Sn1—O1	88.1 (4)
C27—Sn1—N2	93.0 (4)	O3—Sn1—O1	130.3 (3)
C28—Sn1—N2	89.7 (4)	O2—Sn1—O1	52.8 (2)
O3—Sn1—N2	85.6 (3)	N2—Sn1—O1	144.0 (3)
O2—Sn1—N2	163.2 (3)	N1—Sn1—O1	76.4 (3)
C27—Sn1—N1	87.6 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···F5^{i}	0.93	2.48	3.217 (13)	136
C22—H22···O4^{i}	0.93	2.49	3.191 (14)	133

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); 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*.

The authors thank the National Natural Science Foundation of China (grant No. 20271025) and the Natural Science Foundation of Shandong Province for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2474).

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supplementary materials

Acta Cryst. (2007). E**63**, m2691-m2692 [**doi:10.1107/S1600536807048362**]

Dimethyl(1,10-phenanthroline)bis(2,3,4,5-tetrafluorobenzoato)tin(IV)

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Comment

Organotin carboxylate complexes have recently attracted much attention due to their biochemical and commercial applications (Narula *et al.*, 1988). In order to explore the impact of the structure on properties of the complexes, as well as to analyze the structure–activity relationships, a large number of organotin carboxylates have been prepared and studied (Gielen, 2002). We report here the crystal structure of the title compound, $Me_2Sn(C_6HF_4CO_2)_2(C_{12}H_8N_2)$, with 1,10-phenanthroline as a co-ligand.

The coordination geometry about the Sn atom is best described as distorted pentagonal bipyramidal with the axial positions occupied by methyl groups (Table 1). Three carboxylate O atoms (O1,O2,O3) from two tetrafluorobenzoate ligands and the two N atoms (N1,N2) of the 1,10-phenanthroline ligand occupy the basal plane (Fig. 1). The Sn—N distances (Table 1) are longer than the sum of the covalent radii of Sn and N atoms (2.15 Å), but much shorter than the sum of van der Waals radii of the two atoms (3.74 Å; Casas *et al.*, 1997). The Sn1—O3 bond length of 2.146 (7) Å is close to the sum of the covalent radii of Sn and O atoms (2.13 Å), showing strong coordination interaction, which is in agreement with the monodentate coordination mode of the carboxylate group (Li *et al.*, 2005). The Sn1—O2 [2.360 (7) Å] and Sn1—O1 [2.554 (8) Å] distances lie midway between the sums of the van der Waals and covalent radii of Sn and O atoms (2.13–3.68 Å; Ma *et al.*, 2005).

In the crystal structure, C—H···F and C—H···O type hydrogen bonds link the molecules into cyclic centrosymmetric dimers (Table 2).

Experimental

All reagents and solvents were used as obtained without further purification. The reaction was carried out under a nitrogen atmosphere. 2,3,4,5-Tetrafluorobenzoic acid (0.388 g, 2 mmol) was added to a solution of sodium ethoxide (0.272 g, 2 mmol) in benzene (30 ml) and the mixture was stirred for 10 min, after that dimethyltin dichloride (0.220 g, 1 mmol) and 1,10-phenanthroline (0.198 g, 1 mmol) were added. The reaction mixture was kept at 313 K for 12 h. After cooling to room temperature, the solution was filtered. The solvent was removed from the filtrate under vacuum. The solid residue was recrystallized from diethyl ether and colourless crystals of the title compound suitable for X-Ray diffraction studies were obtained (yield 0.724 g, 81%; m.p. 414 K). Analysis, calculated for $C_{28}H_{16}N_2O_4Sn$: C 59.72, H 2.86, N 4.97; found: C 59.53, H 2.68, N 5.17%.

Refinement

H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å (aromatic) and 0.96 Å (methyl) and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$.

Figures

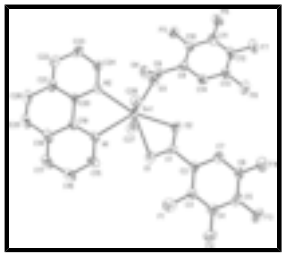


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

Dimethyl(1,10-phenanthroline)bis(2,3,4,5-tetrafluorobenzoato)tin(IV)

Crystal data

$[Sn(CH_3)_2(C_7HF_4O_2)_2(C_{12}H_8N_2)]$	$Z = 2$
$M_r = 715.12$	$F_{000} = 704$
Triclinic, $P\overline{1}$	$D_x = 1.807$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.265$ (4) Å	Cell parameters from 2191 reflections
$b = 10.174$ (6) Å	$\theta = 2.4$–25.8º
$c = 18.957$ (11) Å	$\mu = 1.07$ mm^{-1}
$\alpha = 90.519$ (10)º	$T = 298$ (2) K
$\beta = 90.205$ (9)º	Block, colourless
$\gamma = 110.247$ (8)º	0.18 × 0.13 × 0.09 mm
$V = 1314.5$ (13) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	4483 independent reflections
Radiation source: fine-focus sealed tube	3007 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.054$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.831$, $T_{max} = 0.910$	$k = -12 \rightarrow 11$
6410 measured reflections	$l = -22 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.081$	H-atom parameters constrained
$wR(F^2) = 0.222$	$w = 1/[\sigma^2(F_o^2) + (0.132P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
4483 reflections	$\Delta\rho_{max} = 1.64$ e Å^{-3}
388 parameters	$\Delta\rho_{min} = -2.31$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Sn1	0.23811 (11)	0.21428 (7)	0.24653 (4)	0.0428 (3)
F1	0.6709 (13)	0.3680 (8)	0.4720 (4)	0.089 (2)
F2	0.8879 (12)	0.5751 (8)	0.5510 (4)	0.079 (2)
F3	0.9354 (12)	0.8410 (7)	0.5194 (4)	0.085 (2)
F4	0.7645 (13)	0.8986 (7)	0.4031 (5)	0.095 (3)
F5	0.1948 (11)	0.5064 (7)	−0.0229 (3)	0.0693 (19)
F6	0.2542 (13)	0.7781 (8)	−0.0370 (4)	0.080 (2)
F7	0.3925 (12)	0.9560 (6)	0.0717 (4)	0.076 (2)
F8	0.4790 (11)	0.8624 (7)	0.1952 (4)	0.0697 (19)
N1	0.2041 (13)	−0.0126 (9)	0.3011 (4)	0.048 (2)
N2	0.0471 (13)	0.0191 (8)	0.1755 (5)	0.048 (2)
O1	0.4267 (13)	0.2843 (8)	0.3628 (4)	0.065 (2)
O2	0.4062 (12)	0.4435 (7)	0.2891 (4)	0.063 (2)
O3	0.1802 (11)	0.3414 (7)	0.1657 (4)	0.0480 (17)
O4	0.3100 (14)	0.3174 (8)	0.0624 (4)	0.068 (2)
C1	0.4652 (17)	0.4077 (12)	0.3462 (6)	0.052 (3)
C2	0.5966 (14)	0.5214 (10)	0.3913 (5)	0.042 (2)
C3	0.6878 (16)	0.4988 (10)	0.4510 (6)	0.048 (3)
C4	0.8018 (17)	0.6015 (12)	0.4933 (5)	0.054 (3)
C5	0.8270 (18)	0.7387 (12)	0.4780 (6)	0.063 (3)
C6	0.7380 (17)	0.7658 (10)	0.4181 (6)	0.053 (3)
C7	0.6231 (16)	0.6614 (11)	0.3753 (6)	0.052 (3)
H7	0.5626	0.6825	0.3359	0.062*
C8	0.2614 (17)	0.3861 (11)	0.1077 (6)	0.049 (3)
C9	0.2966 (14)	0.5365 (10)	0.0970 (5)	0.042 (2)
C10	0.2667 (15)	0.5912 (10)	0.0332 (5)	0.045 (2)

C11	0.2951 (18)	0.7302 (12)	0.0255 (6)	0.057 (3)
C12	0.3661 (18)	0.8207 (10)	0.0793 (6)	0.055 (3)
C13	0.4030 (15)	0.7691 (10)	0.1428 (6)	0.046 (2)
C14	0.3653 (15)	0.6309 (11)	0.1512 (6)	0.046 (2)
H14	0.3865	0.5986	0.1952	0.056*
C15	0.2854 (18)	−0.0276 (13)	0.3634 (6)	0.061 (3)
H15	0.3559	0.0518	0.3895	0.073*
C16	0.2661 (19)	−0.1588 (13)	0.3892 (7)	0.066 (3)
H16	0.3235	−0.1667	0.4322	0.079*
C17	0.1632 (18)	−0.2761 (13)	0.3516 (8)	0.069 (4)
H17	0.1506	−0.3639	0.3690	0.083*
C18	0.0780 (19)	−0.2653 (12)	0.2883 (7)	0.061 (3)
C19	0.1024 (14)	−0.1294 (9)	0.2646 (5)	0.040 (2)
C20	0.0178 (14)	−0.1119 (9)	0.1983 (6)	0.043 (2)
C21	−0.0894 (15)	−0.2316 (10)	0.1590 (6)	0.051 (3)
C22	−0.1680 (17)	−0.2121 (12)	0.0942 (6)	0.053 (3)
H22	−0.2387	−0.2886	0.0663	0.064*
C23	−0.1392 (16)	−0.0783 (12)	0.0726 (6)	0.057 (3)
H23	−0.1924	−0.0625	0.0302	0.068*
C24	−0.0302 (17)	0.0321 (12)	0.1148 (6)	0.058 (3)
H24	−0.0101	0.1223	0.0990	0.070*
C25	−0.0352 (18)	−0.3825 (11)	0.2462 (7)	0.064 (3)
H25	−0.0525	−0.4723	0.2619	0.076*
C26	−0.1164 (18)	−0.3679 (11)	0.1858 (7)	0.063 (3)
H26	−0.1917	−0.4470	0.1604	0.076*
C27	0.5007 (19)	0.2137 (12)	0.2044 (6)	0.066 (3)
H27A	0.5862	0.3085	0.1972	0.098*
H27B	0.4758	0.1641	0.1601	0.098*
H27C	0.5617	0.1684	0.2364	0.098*
C28	−0.0154 (18)	0.2079 (12)	0.3005 (6)	0.061 (3)
H28A	−0.0556	0.1281	0.3309	0.092*
H28B	−0.1182	0.2007	0.2672	0.092*
H28C	0.0114	0.2919	0.3283	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0444 (4)	0.0339 (4)	0.0483 (4)	0.0111 (3)	−0.0070 (3)	0.0040 (3)
F1	0.093 (6)	0.073 (5)	0.095 (6)	0.020 (4)	−0.019 (5)	0.006 (4)
F2	0.088 (5)	0.076 (5)	0.061 (4)	0.014 (4)	−0.027 (4)	0.001 (4)
F3	0.088 (6)	0.057 (4)	0.087 (5)	−0.004 (4)	−0.024 (4)	−0.021 (4)
F4	0.115 (7)	0.045 (4)	0.112 (6)	0.011 (4)	−0.020 (5)	0.005 (4)
F5	0.090 (5)	0.055 (4)	0.058 (4)	0.021 (4)	−0.019 (4)	−0.008 (3)
F6	0.110 (6)	0.066 (5)	0.073 (4)	0.043 (4)	−0.012 (4)	0.015 (4)
F7	0.098 (6)	0.038 (3)	0.095 (5)	0.026 (4)	0.015 (4)	0.011 (3)
F8	0.075 (5)	0.050 (4)	0.078 (4)	0.014 (3)	0.003 (4)	−0.017 (3)
N1	0.053 (5)	0.043 (5)	0.054 (5)	0.023 (4)	0.000 (4)	0.015 (4)
N2	0.051 (5)	0.035 (4)	0.060 (6)	0.016 (4)	−0.008 (4)	0.000 (4)

O1	0.072 (6)	0.041 (4)	0.076 (5)	0.013 (4)	−0.014 (4)	−0.002 (4)
O2	0.069 (5)	0.041 (4)	0.060 (5)	−0.002 (4)	−0.023 (4)	−0.002 (4)
O3	0.054 (4)	0.042 (4)	0.047 (4)	0.016 (3)	−0.001 (4)	0.009 (3)
O4	0.089 (6)	0.047 (5)	0.066 (5)	0.021 (4)	0.009 (5)	0.004 (4)
C1	0.055 (7)	0.051 (7)	0.048 (6)	0.017 (5)	−0.022 (5)	−0.005 (5)
C2	0.036 (5)	0.035 (5)	0.054 (6)	0.011 (4)	0.002 (5)	−0.006 (5)
C3	0.053 (6)	0.031 (5)	0.054 (6)	0.006 (5)	0.000 (5)	0.007 (5)
C4	0.057 (7)	0.060 (7)	0.041 (6)	0.014 (6)	−0.004 (5)	−0.002 (5)
C5	0.064 (8)	0.051 (7)	0.057 (7)	0.000 (6)	−0.004 (6)	−0.012 (6)
C6	0.054 (7)	0.029 (5)	0.068 (7)	0.003 (5)	0.003 (6)	0.004 (5)
C7	0.043 (6)	0.044 (6)	0.062 (7)	0.006 (5)	−0.003 (5)	0.001 (5)
C8	0.055 (7)	0.040 (6)	0.046 (6)	0.011 (5)	−0.012 (5)	−0.005 (5)
C9	0.037 (5)	0.042 (5)	0.047 (6)	0.012 (4)	−0.002 (5)	0.005 (5)
C10	0.044 (6)	0.044 (6)	0.045 (6)	0.014 (5)	0.004 (5)	0.001 (5)
C11	0.064 (7)	0.050 (7)	0.058 (7)	0.019 (6)	0.008 (6)	0.014 (6)
C12	0.063 (7)	0.031 (5)	0.071 (7)	0.016 (5)	0.010 (6)	0.009 (5)
C13	0.038 (6)	0.040 (5)	0.062 (7)	0.016 (5)	0.008 (5)	−0.004 (5)
C14	0.037 (5)	0.050 (6)	0.052 (6)	0.015 (5)	0.007 (5)	0.004 (5)
C15	0.055 (7)	0.069 (8)	0.072 (8)	0.037 (6)	−0.005 (6)	0.012 (6)
C16	0.063 (8)	0.065 (8)	0.081 (8)	0.037 (7)	0.006 (7)	0.026 (7)
C17	0.050 (7)	0.060 (8)	0.108 (11)	0.032 (6)	0.016 (7)	0.034 (7)
C18	0.066 (8)	0.044 (6)	0.071 (8)	0.015 (6)	0.018 (6)	0.021 (6)
C19	0.034 (5)	0.024 (4)	0.063 (6)	0.012 (4)	0.005 (5)	0.009 (4)
C20	0.032 (5)	0.023 (5)	0.065 (7)	0.000 (4)	0.008 (5)	0.006 (4)
C21	0.032 (5)	0.038 (6)	0.075 (8)	−0.001 (4)	0.016 (5)	−0.001 (5)
C22	0.049 (6)	0.048 (6)	0.056 (7)	0.010 (5)	0.005 (5)	−0.008 (5)
C23	0.046 (6)	0.051 (7)	0.057 (7)	−0.003 (5)	−0.004 (5)	−0.001 (5)
C24	0.064 (7)	0.040 (6)	0.055 (7)	0.000 (5)	−0.011 (6)	0.008 (5)
C25	0.065 (8)	0.031 (6)	0.098 (10)	0.021 (5)	0.015 (7)	0.013 (6)
C26	0.059 (7)	0.028 (5)	0.095 (9)	0.006 (5)	0.021 (7)	0.002 (6)
C27	0.072 (8)	0.050 (7)	0.070 (8)	0.016 (6)	−0.012 (7)	−0.010 (6)
C28	0.068 (8)	0.045 (6)	0.065 (7)	0.011 (6)	−0.004 (6)	0.009 (5)

Geometric parameters (Å, °)

Sn1—C27	2.072 (13)	C9—C10	1.382 (14)
Sn1—C28	2.092 (13)	C10—C11	1.366 (15)
Sn1—O3	2.146 (7)	C11—C12	1.344 (16)
Sn1—O2	2.360 (7)	C12—C13	1.380 (16)
Sn1—N2	2.389 (8)	C13—C14	1.348 (14)
Sn1—N1	2.472 (8)	C14—H14	0.93
Sn1—O1	2.554 (8)	C15—C16	1.388 (16)
F1—C3	1.356 (12)	C15—H15	0.93
F2—C4	1.332 (12)	C16—C17	1.361 (18)
F3—C5	1.317 (12)	C16—H16	0.93
F4—C6	1.331 (12)	C17—C18	1.371 (17)
F5—C10	1.347 (11)	C17—H17	0.93
F6—C11	1.355 (13)	C18—C19	1.410 (14)
F7—C12	1.332 (11)	C18—C25	1.426 (17)

F8—C13	1.345 (11)	C19—C20	1.436 (14)
N1—C19	1.346 (12)	C20—C21	1.403 (13)
N1—C15	1.351 (14)	C21—C22	1.397 (16)
N2—C24	1.307 (13)	C21—C26	1.430 (16)
N2—C20	1.350 (12)	C22—C23	1.370 (16)
O1—C1	1.232 (13)	C22—H22	0.93
O2—C1	1.265 (12)	C23—C24	1.376 (14)
O3—C8	1.261 (13)	C23—H23	0.93
O4—C8	1.229 (13)	C24—H24	0.93
C1—C2	1.481 (14)	C25—C26	1.319 (17)
C2—C3	1.371 (14)	C25—H25	0.93
C2—C7	1.406 (14)	C26—H26	0.93
C3—C4	1.343 (14)	C27—H27A	0.96
C4—C5	1.378 (16)	C27—H27B	0.96
C5—C6	1.380 (16)	C27—H27C	0.96
C6—C7	1.359 (14)	C28—H28A	0.96
C7—H7	0.93	C28—H28B	0.96
C8—C9	1.478 (14)	C28—H28C	0.96
C9—C14	1.370 (14)		
C27—Sn1—C28	173.1 (4)	C12—C11—F6	119.5 (10)
C27—Sn1—O3	95.4 (4)	C12—C11—C10	120.4 (10)
C28—Sn1—O3	91.1 (4)	F6—C11—C10	120.1 (10)
C27—Sn1—O2	88.2 (4)	F7—C12—C11	120.2 (11)
C28—Sn1—O2	90.9 (4)	F7—C12—C13	121.3 (10)
O3—Sn1—O2	77.6 (3)	C11—C12—C13	118.4 (10)
C27—Sn1—N2	93.0 (4)	F8—C13—C14	121.8 (10)
C28—Sn1—N2	89.7 (4)	F8—C13—C12	117.3 (9)
O3—Sn1—N2	85.6 (3)	C14—C13—C12	120.9 (10)
O2—Sn1—N2	163.2 (3)	C13—C14—C9	121.9 (10)
C27—Sn1—N1	87.6 (4)	C13—C14—H14	119.0
C28—Sn1—N1	87.6 (4)	C9—C14—H14	119.0
O3—Sn1—N1	153.2 (3)	N1—C15—C16	121.5 (12)
O2—Sn1—N1	129.2 (3)	N1—C15—H15	119.3
N2—Sn1—N1	67.6 (3)	C16—C15—H15	119.3
C27—Sn1—O1	85.9 (4)	C17—C16—C15	119.9 (12)
C28—Sn1—O1	88.1 (4)	C17—C16—H16	120.0
O3—Sn1—O1	130.3 (3)	C15—C16—H16	120.0
O2—Sn1—O1	52.8 (2)	C16—C17—C18	120.4 (11)
N2—Sn1—O1	144.0 (3)	C16—C17—H17	119.8
N1—Sn1—O1	76.4 (3)	C18—C17—H17	119.8
C19—N1—C15	118.0 (9)	C17—C18—C19	117.3 (11)
C19—N1—Sn1	117.1 (6)	C17—C18—C25	124.1 (11)
C15—N1—Sn1	124.9 (8)	C19—C18—C25	118.6 (11)
C24—N2—C20	117.6 (9)	N1—C19—C18	123.0 (10)
C24—N2—Sn1	123.4 (7)	N1—C19—C20	117.3 (8)
C20—N2—Sn1	119.1 (7)	C18—C19—C20	119.7 (9)
C1—O1—Sn1	88.1 (6)	N2—C20—C21	122.4 (10)
C1—O2—Sn1	96.3 (7)	N2—C20—C19	118.9 (8)
C8—O3—Sn1	133.0 (7)	C21—C20—C19	118.7 (9)

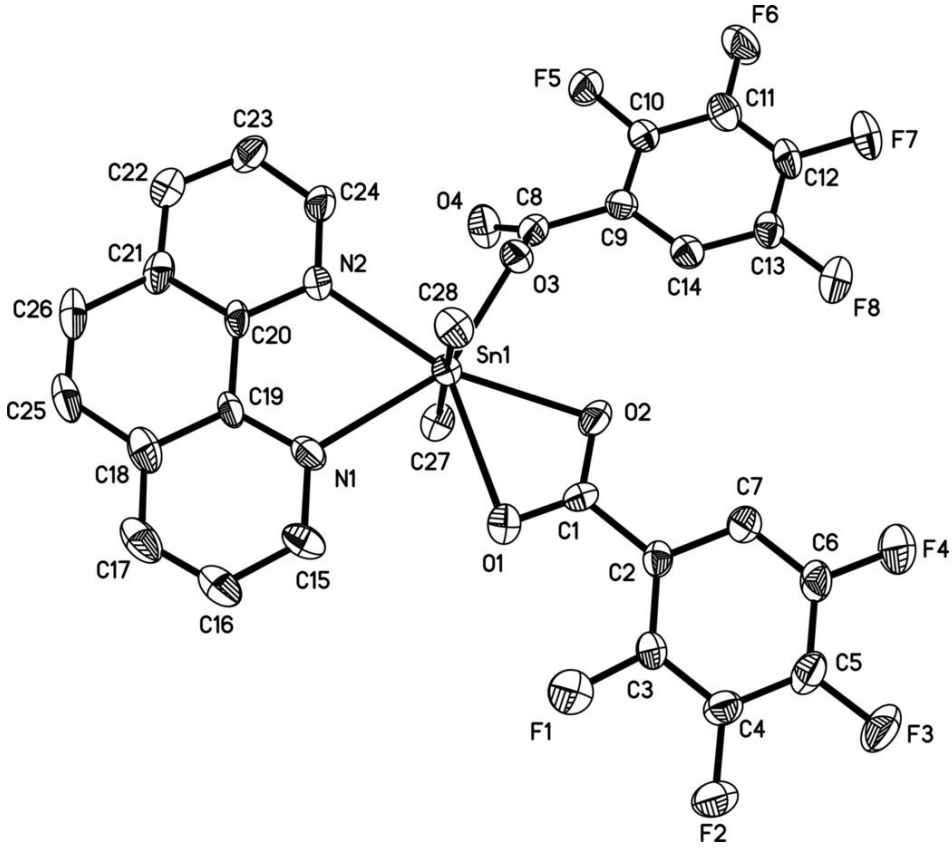
O1—C1—O2	122.8 (10)	C22—C21—C20	117.8 (10)
O1—C1—C2	120.2 (9)	C22—C21—C26	122.2 (10)
O2—C1—C2	116.9 (10)	C20—C21—C26	120.0 (11)
C3—C2—C7	116.8 (9)	C23—C22—C21	118.9 (10)
C3—C2—C1	123.8 (9)	C23—C22—H22	120.6
C7—C2—C1	119.3 (10)	C21—C22—H22	120.6
C4—C3—F1	114.1 (9)	C22—C23—C24	118.8 (11)
C4—C3—C2	124.0 (10)	C22—C23—H23	120.6
F1—C3—C2	121.9 (9)	C24—C23—H23	120.6
F2—C4—C3	122.1 (11)	N2—C24—C23	124.6 (11)
F2—C4—C5	118.6 (10)	N2—C24—H24	117.7
C3—C4—C5	119.2 (10)	C23—C24—H24	117.7
F3—C5—C4	120.2 (11)	C26—C25—C18	122.3 (11)
F3—C5—C6	121.3 (11)	C26—C25—H25	118.9
C4—C5—C6	118.5 (10)	C18—C25—H25	118.9
F4—C6—C7	119.7 (11)	C25—C26—C21	120.6 (11)
F4—C6—C5	118.3 (10)	C25—C26—H26	119.7
C7—C6—C5	122.0 (10)	C21—C26—H26	119.7
C6—C7—C2	119.4 (10)	Sn1—C27—H27A	109.5
C6—C7—H7	120.3	Sn1—C27—H27B	109.5
C2—C7—H7	120.3	H27A—C27—H27B	109.5
O4—C8—O3	126.4 (10)	Sn1—C27—H27C	109.5
O4—C8—C9	120.3 (10)	H27A—C27—H27C	109.5
O3—C8—C9	113.2 (9)	H27B—C27—H27C	109.5
C14—C9—C10	116.1 (10)	Sn1—C28—H28A	109.5
C14—C9—C8	120.4 (9)	Sn1—C28—H28B	109.5
C10—C9—C8	123.5 (9)	H28A—C28—H28B	109.5
F5—C10—C11	117.2 (10)	Sn1—C28—H28C	109.5
F5—C10—C9	120.6 (9)	H28A—C28—H28C	109.5
C11—C10—C9	122.1 (10)	H28B—C28—H28C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···F5^{i}	0.93	2.48	3.217 (13)	136
C22—H22···O4^{i}	0.93	2.49	3.191 (14)	133

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1


F6
F5
C10
C11
F7
C23
C22
C24
C12
O4
C8
C9
C21
N2
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C14
C13
F8
C26
C28
C20
Sn1
C25
C19
O2
C27
C18
N1
C7
C1
C6
F4
C17
C15
O1
C2
C16
C5
C3
F1
C4
F3
F2