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Bis(chloroacetato-κ^2O,O')bis(2-fluorobenzyl-κC^1)tin(IV)

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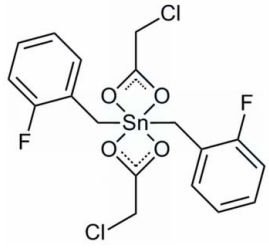
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.071; data-to-parameter ratio = 14.3.

In the title complex, $[Sn(C_2H_2ClO_2)_2(C_7H_6F)_2]$, the Sn^{IV} atom is located on a twofold rotation axis and forms a strongly distorted *trans*-octahedral geometry. The equatorial plane is defined by two chelating chloroacetate ligands with asymmetrical Sn—O bond lengths, while the axial positions are occupied by the C atoms of two 2-fluorobenzyl groups. In the crystal, infinite chains in the [010] direction are formed through intermolecular Sn···O interactions [Sn···O separation = 3.682 (3) Å].

Related literature

For details of the synthesis, see: Zhang *et al.* (2007).



Experimental

Crystal data

$[Sn(C_2H_2ClO_2)_2(C_7H_6F)_2]$
M_r = 523.90
Monoclinic, $C2/c$
a = 17.3841 (18) Å
b = 5.0480 (8) Å
c = 22.808 (2) Å
β = 93.760 (1)°
V = 1997.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 298 K
0.29 × 0.15 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.656, T_{max} = 0.833
4738 measured reflections
1754 independent reflections
1551 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.071
S = 1.00
1754 reflections
123 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O1	2.109 (2)	Sn1—O2	2.537 (3)
Sn1—C3	2.121 (4)		

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: BH2395).

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Zhang, J.-H., Ma, C.-L. & Zhang, R.-F. (2007). *Acta Cryst.* E**63**, m2161.

supporting information

Acta Cryst. (2011). E**67**, m1905 [https://doi.org/10.1107/S1600536811051002]

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S1. Comment

The title complex was obtained using a route similar to that used for the synthesis of a trinuclear tin complex (Zhang *et al.*, 2007). The title complex has 2-fold symmetry, with the Sn atom placed on the crystallographic symmetry axis (Fig. 1). Selected bond lengths and angles are given in table 1. The coordination geometry of tin can be described as a distorted *trans*-octahedron geometry, with two C atoms of 2-fluorobenzyl groups occupying the axial positions. The C3—Sn1—C3^i bond angle of 133.6 (2)° (symmetry code *i*: 1 - *x*, *y*, 1/2 - *z*) reflects the distortion from octahedral geometry. The equatorial plane is defined by four O atoms of two symmetry-related chloroacetate ligands. The bond lengths in the equatorial plane are Sn1—O1 = 2.109 (2) and Sn1—O2 = 2.537 (3) Å, reflecting the asymmetrical coordination of acetate groups.

The complex forms infinite chains containing Sn_2O_2 rings, through intermolecular Sn···O contacts, characterized by separations Sn···O = 3.682 (3) Å (Fig. 2).

S2. Experimental

Chloroacetic acid (2 mmol) was added to a sodium ethoxide solution (2 mmol, 20 ml of ethanol), and the mixture was stirred for 30 min. Then, 1 mmol of bis(2-fluorobenzyl)tin(IV)dichloride (Zhang *et al.*, 2007) was added to the mixture, continuing the reaction for 12 h at 318 K. After cooling down to room temperature, the reaction was filtered off. The solvent of the filtrate was gradually removed by evaporation under vacuum, until a solid product was obtained. The solid was recrystallized from ether-dichloromethane and colourless crystals suitable for X-ray diffraction were obtained (m.p. 464 K). Analysis calculated for $C_{18}H_{16}Cl_2F_2O_4Sn$: C 41.26, H 3.08%; found: C 41.29, H 3.06%.

S3. Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with C—H bond lengths fixed to 0.93 Å for aromatic CH and 0.97 Å for methylene CH_2. Isotropic displacement parameters for H atoms were calculated as U_{iso}(H) = 1.2U_{eq}(carrier C).

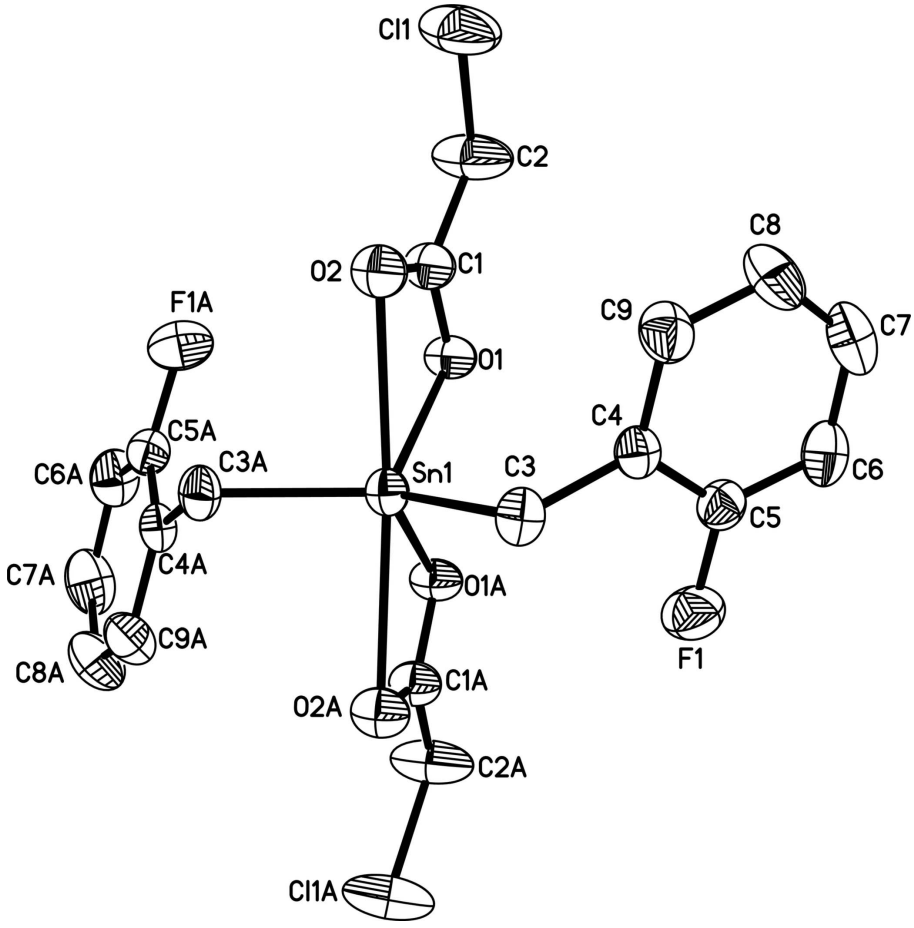

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

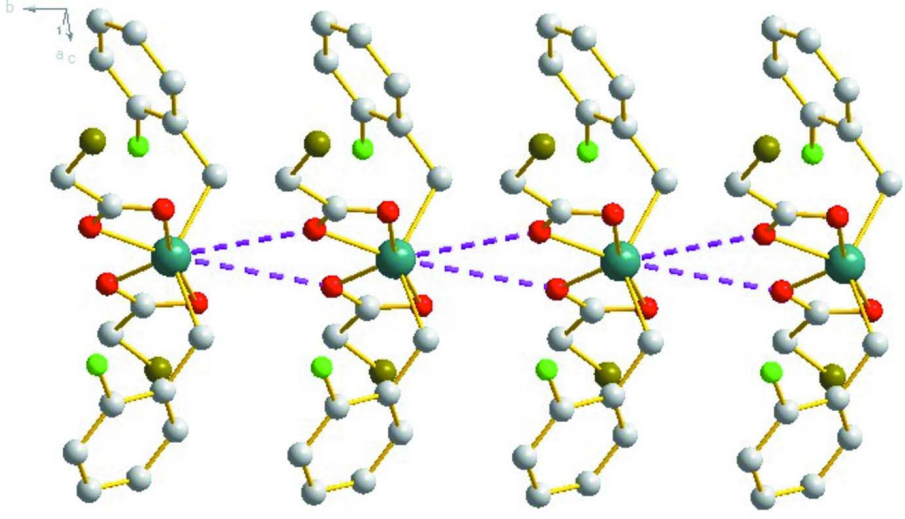

Figure 2

The unit cell of the title compound.

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Crystal data

$[Sn(C_2H_2ClO_2)_2(C_7H_6F)_2]$
$M_r = 523.90$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 17.3841\ (18)$ Å
$b = 5.0480\ (8)$ Å
$c = 22.808\ (2)$ Å
$\beta = 93.760\ (1)°$
$V = 1997.2\ (4)$ Å^3
$Z = 4$
$F(000) = 1032$
$D_x = 1.742$ Mg m^{-3}
Melting point: 464 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1705 reflections
$\theta = 2.9–25.0°$
$\mu = 1.59$ mm^{-1}
$T = 298$ K
Block, colourless
0.29 × 0.15 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.656$, $T_{max} = 0.833$
4738 measured reflections
1754 independent reflections
1551 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -20\rightarrow17$
$k = -5\rightarrow6$
$l = -27\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.071$
$S = 1.00$
1754 reflections
123 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.5000	0.07163 (7)	0.2500	0.04380 (15)
Cl1	0.58874 (11)	0.2741 (3)	0.03745 (5)	0.1169 (6)
F1	0.29621 (15)	0.3089 (6)	0.24062 (11)	0.0831 (8)
O1	0.52467 (15)	0.3929 (5)	0.19515 (10)	0.0517 (7)
O2	0.55526 (17)	0.0310 (5)	0.15017 (12)	0.0602 (7)
C1	0.5493 (2)	0.2692 (9)	0.15046 (17)	0.0542 (10)
C2	0.5669 (4)	0.4449 (10)	0.0999 (2)	0.098 (2)
H2A	0.6101	0.5583	0.1120	0.117*
H2B	0.5227	0.5579	0.0903	0.117*
C3	0.3963 (2)	−0.0939 (7)	0.21189 (17)	0.0522 (10)
H3A	0.4080	−0.2616	0.1937	0.063*
H3B	0.3620	−0.1296	0.2428	0.063*

C4	0.3557 (2)	0.0799 (8)	0.16691 (16)	0.0465 (9)
C5	0.3052 (2)	0.2743 (9)	0.18211 (18)	0.0537 (10)
C6	0.2662 (3)	0.4379 (9)	0.1434 (2)	0.0703 (13)
H6	0.2318	0.5635	0.1561	0.084*
C7	0.2789 (3)	0.4122 (11)	0.0846 (2)	0.0820 (15)
H7	0.2537	0.5231	0.0570	0.098*
C8	0.3286 (3)	0.2242 (12)	0.0670 (2)	0.0863 (16)
H8	0.3370	0.2078	0.0273	0.104*
C9	0.3667 (3)	0.0579 (10)	0.10703 (19)	0.0683 (12)
H9	0.4000	−0.0703	0.0940	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0453 (2)	0.0360 (2)	0.0496 (2)	0.000	−0.00011 (16)	0.000
Cl1	0.1927 (17)	0.1008 (12)	0.0620 (8)	0.0479 (12)	0.0451 (10)	0.0020 (8)
F1	0.0875 (19)	0.084 (2)	0.0804 (18)	0.0152 (16)	0.0270 (15)	0.0010 (15)
O1	0.0685 (18)	0.0384 (16)	0.0496 (15)	0.0031 (13)	0.0147 (13)	0.0003 (12)
O2	0.078 (2)	0.0402 (17)	0.0635 (17)	0.0078 (14)	0.0121 (15)	0.0013 (13)
C1	0.065 (3)	0.046 (3)	0.052 (2)	0.003 (2)	0.010 (2)	0.001 (2)
C2	0.171 (6)	0.058 (3)	0.071 (3)	0.017 (4)	0.057 (4)	0.005 (3)
C3	0.049 (2)	0.039 (2)	0.068 (3)	−0.0047 (19)	−0.0033 (19)	−0.004 (2)
C4	0.043 (2)	0.043 (2)	0.053 (2)	−0.0078 (19)	−0.0053 (17)	−0.0040 (19)
C5	0.047 (2)	0.057 (3)	0.057 (3)	−0.003 (2)	0.003 (2)	−0.003 (2)
C6	0.058 (3)	0.062 (3)	0.089 (4)	0.014 (2)	−0.008 (2)	−0.002 (3)
C7	0.085 (4)	0.072 (4)	0.084 (4)	0.003 (3)	−0.032 (3)	0.012 (3)
C8	0.105 (4)	0.098 (4)	0.052 (3)	0.002 (4)	−0.022 (3)	−0.003 (3)
C9	0.071 (3)	0.072 (3)	0.060 (3)	0.008 (3)	−0.008 (2)	−0.016 (2)

Geometric parameters (Å, º)

Sn1—O1^{i}	2.109 (2)	C3—C4	1.492 (5)
Sn1—O1	2.109 (2)	C3—H3A	0.9700
Sn1—C3	2.121 (4)	C3—H3B	0.9700
Sn1—C3^{i}	2.121 (4)	C4—C5	1.375 (5)
Sn1—O2^{i}	2.537 (3)	C4—C9	1.396 (6)
Sn1—O2	2.537 (3)	C5—C6	1.359 (6)
Cl1—C2	1.728 (5)	C6—C7	1.380 (7)
F1—C5	1.365 (4)	C6—H6	0.9300
O1—C1	1.292 (4)	C7—C8	1.361 (7)
O2—C1	1.207 (4)	C7—H7	0.9300
C1—C2	1.503 (6)	C8—C9	1.377 (7)
C2—H2A	0.9700	C8—H8	0.9300
C2—H2B	0.9700	C9—H9	0.9300
O1^{i}—Sn1—O1	79.50 (13)	H2A—C2—H2B	107.7
O1^{i}—Sn1—C3	110.21 (13)	C4—C3—Sn1	113.7 (3)
O1—Sn1—C3	105.08 (12)	C4—C3—H3A	108.8

O1^{i}—Sn1—C3^{i}	105.08 (12)	Sn1—C3—H3A	108.8
O1—Sn1—C3^{i}	110.21 (13)	C4—C3—H3B	108.8
C3—Sn1—C3^{i}	133.6 (2)	Sn1—C3—H3B	108.8
O1^{i}—Sn1—O2^{i}	54.99 (9)	H3A—C3—H3B	107.7
O1—Sn1—O2^{i}	134.28 (9)	C5—C4—C9	115.7 (4)
C3—Sn1—O2^{i}	88.52 (13)	C5—C4—C3	121.8 (3)
C3^{i}—Sn1—O2^{i}	87.82 (13)	C9—C4—C3	122.5 (4)
O1^{i}—Sn1—O2	134.28 (9)	C6—C5—F1	118.2 (4)
O1—Sn1—O2	54.99 (9)	C6—C5—C4	124.7 (4)
C3—Sn1—O2	87.82 (13)	F1—C5—C4	117.0 (4)
C3^{i}—Sn1—O2	88.52 (13)	C5—C6—C7	118.0 (4)
O2^{i}—Sn1—O2	170.72 (12)	C5—C6—H6	121.0
C1—O1—Sn1	100.8 (2)	C7—C6—H6	121.0
C1—O2—Sn1	82.9 (2)	C8—C7—C6	119.8 (5)
O2—C1—O1	121.3 (4)	C8—C7—H7	120.1
O2—C1—C2	124.2 (4)	C6—C7—H7	120.1
O1—C1—C2	114.5 (4)	C7—C8—C9	121.1 (5)
C1—C2—Cl1	113.9 (3)	C7—C8—H8	119.5
C1—C2—H2A	108.8	C9—C8—H8	119.5
Cl1—C2—H2A	108.8	C8—C9—C4	120.6 (4)
C1—C2—H2B	108.8	C8—C9—H9	119.7
Cl1—C2—H2B	108.8	C4—C9—H9	119.7

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