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Dicyclohexylammonium bis(chlorodifluoroacetato-κO)cyclopentyldiphenylstannate(IV)

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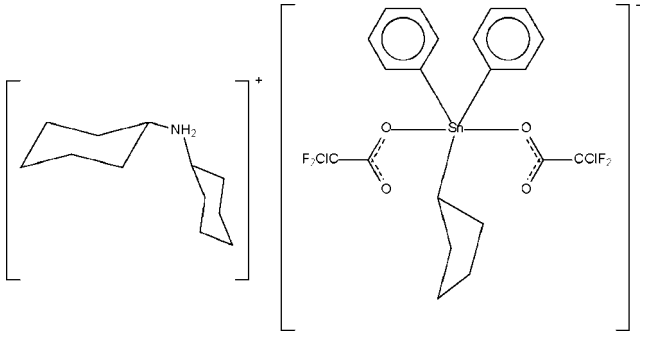
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.010 Å; disorder in main residue; R factor = 0.050; wR factor = 0.133; data-to-parameter ratio = 18.6.

The five-coordinate Sn atom in the title mixed organyl stannate compound, $(C_{12}H_{24}N)[Sn(C_5H_9)(C_6H_5)_2(C_2ClF_2O_2)]$, is in a *trans*-$C_3SnO_2$ trigonal–bipyramidal coordination environment. The NH_2 groups of the cations act as hydrogen-bond donors to two symmetry-related anions, resulting in the formation of linear chains. One of the phenyl rings is disordered over two sites with equal occupancies.

Related literature

For details of the crystal structure of dicyclohexylammonium bis(chlorodifluoroacetato)cyclohexyldiphenylstannate(IV), see Teo *et al.* (2008). For a review of the structural chemistry of organotin carboxylates, see: Tiekink (1991, 1994).



Experimental

Crystal data

$(C_{12}H_{24}N)[Sn(C_5H_9)(C_6H_5)_2(C_2ClF_2O_2)]$
M_r = 783.27
Monoclinic, $P2_1$
a = 8.8610 (2) Å
b = 19.3132 (3) Å
c = 10.6823 (2) Å
β = 109.385 (1)°
V = 1724.47 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.679, T_{max} = 0.870
18017 measured reflections
7831 independent reflections
6637 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.132
S = 1.04
7831 reflections
421 parameters
41 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Flack (1983), 3766 Friedel pairs
Flack parameter: −0.03 (3)

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.147 (5)	Sn1—O1	2.287 (4)
Sn1—C7	2.136 (6)	Sn1—O3	2.249 (4)
Sn1—C13	2.117 (6)		
C1—Sn1—C7	119.2 (2)	C7—Sn1—O1	90.6 (2)
C1—Sn1—C13	121.7 (2)	C7—Sn1—O3	87.8 (2)
C1—Sn1—O1	91.3 (2)	C13—Sn1—O1	82.8 (3)
C1—Sn1—O3	90.9 (2)	C13—Sn1—O3	96.5 (3)
C7—Sn1—C13	118.9 (2)	O1—Sn1—O3	177.7 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O2	0.88	1.88	2.758 (6)	173
N1—H1*N*2···O4^{i}	0.88	1.93	2.804 (6)	169

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

Data collection: *APEX2* (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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2611).

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