

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# Dicyclohexylammonium bis(chloro-difluoroacetato- $\kappa$ O)cyclopentyl-diphenylstannate(IV)

Yin Yin Teo, Kong Mun Lo and Seik Weng Ng\*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

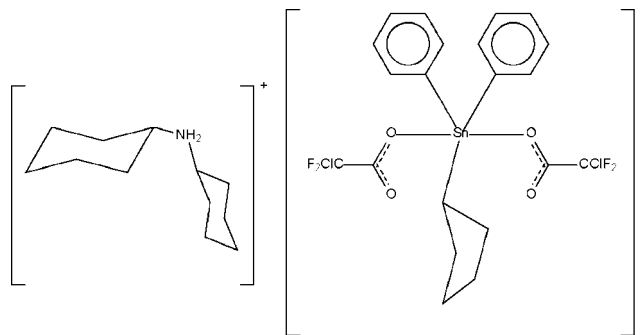
Received 1 April 2008; accepted 18 April 2008

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.010$  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,  $(\text{C}_{12}\text{H}_{24}\text{N})[\text{Sn}(\text{C}_5\text{H}_9)(\text{C}_6\text{H}_5)_2(\text{C}_2\text{ClF}_2\text{O}_2)]$ , is in a *trans*- $\text{C}_3\text{SnO}_2$  trigonal-bipyramidal coordination environment. The  $\text{NH}_2$  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

 $(\text{C}_{12}\text{H}_{24}\text{N})[\text{Sn}(\text{C}_5\text{H}_9)(\text{C}_6\text{H}_5)_2(\text{C}_2\text{ClF}_2\text{O}_2)]$ 
 $M_r = 783.27$ Monoclinic,  $P2_1$  $a = 8.8610$  (2) Å $b = 19.3132$  (3) Å $c = 10.6823$  (2) Å $\beta = 109.385$  (1)° $V = 1724.47$  (6) Å<sup>3</sup> $Z = 2$ Mo  $K\alpha$  radiation $\mu = 0.95$  mm<sup>-1</sup> $T = 100$  (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  $I > 2\sigma(I)$  $R_{\text{int}} = 0.038$ 

### 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

 $\Delta\rho_{\text{max}} = 1.11$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.71$  e Å<sup>-3</sup>

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, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N1 $\cdots$ O2	0.88	1.88	2.758 (6)	173
N1—H1N2 $\cdots$ O4 <sup>i</sup>	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).

The authors thank the University of Malaya for funding this study (grant No. SF022155/2007A) and also for the purchase of the diffractometer.

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

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