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Bis(3-carboxyanilinium) hexafluorostannate(IV)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.063
Data-to-parameter ratio = 17.4

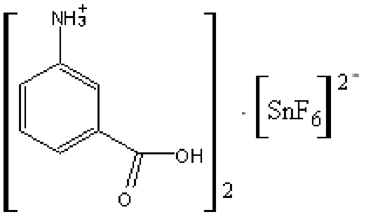
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $(C_7H_8NO_2)_2[SnF_6]$, has been prepared from 3-aminobenzoic acid and tin(II) fluoride in hydrofluoric acid. The structure can be described as alternating layers of SnF_6^{2-} and $C_7H_8NO_2^+$ ions along the a axis, with the SnF_6^{2-} ions lying on a twofold axis. The cations and anions are linked to each other through strong hydrogen bonds formed by all H atoms covalently bonded to the N and O atoms. This three-dimensional complex network of hydrogen bonds reinforces the cohesion of the ionic structure.

Comment

Organic–inorganic hybrid materials have attracted a great deal of attention over the past few decades (Koutselas *et al.*, 1996; Mitzi *et al.*, 1998; Mayer *et al.*, 1999; Mazeaud *et al.*, 2000) because of their ionic, electrical, magnetic and optical properties (Hill, 1998; Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002).

The structural characteristics of compounds with the formula $(RNH_3)_2[SnX_6]$ (where X is Cl, F, Br or I) have not been investigated extensively. The crystal structures of only four primary n-alkylammonium hexachlorostannate(IV) compounds, with chain lengths ranging from one to four, have been reported in the literature to date (Kitahama *et al.*, 1979; Knop *et al.*, 1983; Elleuch *et al.*, 1996). Only one crystal structure of an arylammonium hexachlorostannate(IV) compound has been reported previously (Rademeyer, 2004). In this study, we present a new organic–inorganic hybrid compound of the type $(RNH_3)_2[SnX_6]$, which promises both the superior carrier mobility of inorganic semiconductors and the processability of organic materials.



(I)

The title structure, (I), contains anionic sheets of formula $[SnF_6]^{2-}$ parallel to the (100) plane; the distance between two sheets is a/2 and charge compensation is achieved by the incorporation of the protonated amine of 3-aminobenzoic acid. There are two crystallographically equivalent (3-carboxyanilinium) cations in (I). The asymmetric unit contains 15 non-H atoms, with atoms Sn, F1 and F4 lying on a crystallographic twofold axis in special positions $(0, -y, \frac{3}{4})$. The molecular geometry and atom-numbering scheme used are shown in Fig. 1. The benzene ring of the 3-carboxyanilinium

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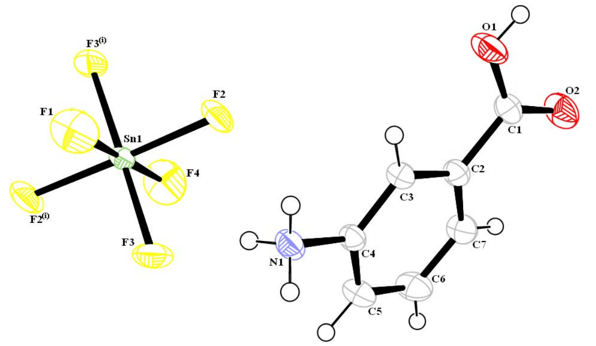

Figure 1
ORTEP-3 view (Farrugia, 1997) of the anion and cation of the title compound, showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $2 - x$, y, $\frac{3}{2} - z$.]

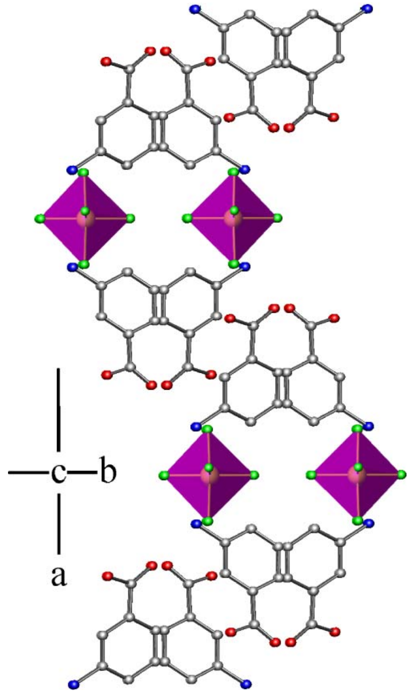

Figure 2
ATOMS diagram (Dowty, 1995) of the layered packing and octahedra in the title compound, viewed down the *c* axis.

cation and atoms C1 and N1 are coplanar. The cations form zigzag layers parallel to the (101) plane. The Sn atom is six-coordinated and forms a quasi-regular octahedral arrangement. The $[SnF_6]^{2-}$ octahedra in (I) alternate with cationic layers along the *a* axis. The tilted octahedra and layered packing are illustrated in Fig. 2.

In this structure, two types of hydrogen bonds are observed, *viz*. cation–cation and cation–anion (Fig. 3). The Sn—F bond lengths for the F atoms engaged in strong hydrogen bonding with the ammonium group and cations are linked by C—H···O and N—H···O hydrogen bonds. The carboxylic acid group is not deprotonated and its H atom is involved in the strongest interaction with the hexafluorostannate anion [O1—H1···F2 = 2.551 (2) Å]. Additional hydrogen-bonding parameters are listed in Table 2.

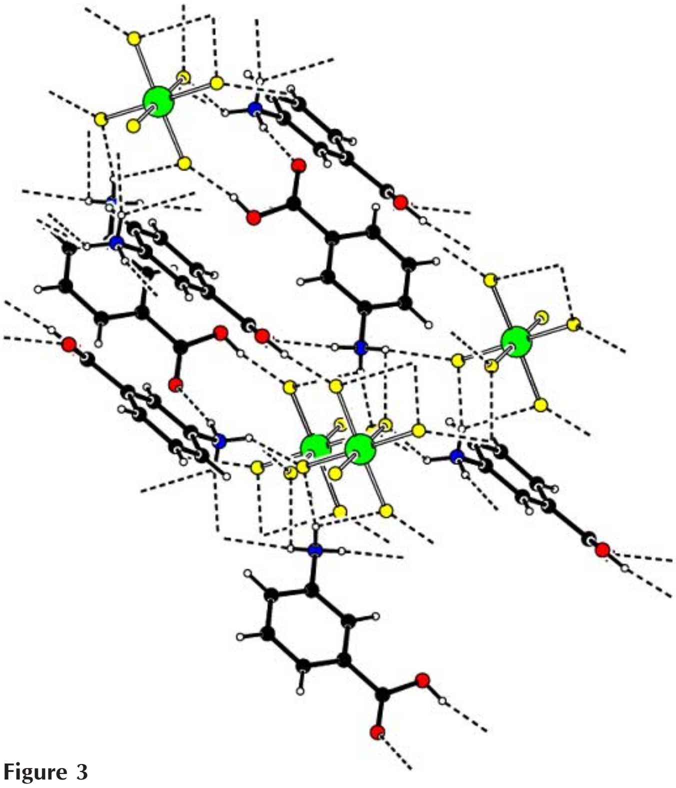

Figure 3
PLUTON view (Spek, 2003) of the ionic stacking, showing the three-dimensional network of hydrogen bonds as dashed lines.

Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of 3-aminobenzoic acid, tin(II) fluoride and hydrofluoric acid in a molar ratio of 10:5:1. After five weeks, brown crystals were obtained and were manually separated under a polarizing microscope.

Crystal data

$(C_7H_8NO_2)_2[SnF_6]$
$M_r = 508.98$
Monoclinic, $C2/c$
$a = 22.2660$ (5) Å
$b = 10.6580$ (5) Å
$c = 7.4920$ (5) Å
$\beta = 103.743$ (5)°
$V = 1727.03$ (15) Å^3
$Z = 4$
$D_x = 1.958$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8090 reflections
$\theta = 1.9$–30.0°
$\mu = 1.57$ mm^{-1}
$T = 295$ (2) K
Needle, brown
0.35 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: none
8090 measured reflections
2517 independent reflections
2291 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\rm max} = 30.0°$
$h = -23 \rightarrow 31$
$k = -14 \rightarrow 12$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.063$
$S = 1.10$
2517 reflections
145 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.66$ e Å^{-3}
$\Delta\rho_{\rm min} = -1.11$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—F1	1.927 (2)	O2—C1	1.214 (3)
Sn1—F4	1.934 (2)	O1—C1	1.311 (3)
Sn1—F3	1.9622 (13)	N1—C4	1.466 (3)
Sn1—F2	1.9654 (14)	C2—C1	1.491 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···F2^{i}	0.82	1.74	2.551 (2)	169
N1—H11···O2^{ii}	0.89 (3)	2.07 (3)	2.942 (3)	166 (3)
N1—H12···F2	0.83 (3)	2.51 (3)	3.008 (3)	119 (3)
N1—H12···F3	0.83 (3)	1.98 (3)	2.804 (3)	167 (3)
N1—H13···F3^{iii}	0.87 (3)	2.10 (3)	2.834 (3)	141 (3)
N1—H13···F1^{iv}	0.87 (3)	2.36 (3)	2.757 (2)	108 (2)
C3—H3···O2^{ii}	0.94 (3)	2.55 (3)	3.335 (3)	140 (3)
C5—H5···F3^{iii}	0.93 (3)	2.44 (3)	3.094 (3)	128 (2)

Symmetry codes: (i) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$; (ii) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $2 - x, y, \frac{1}{2} - z$; (iv) $2 - x, 1 - y, 1 - z$.

All H atoms were located in difference Fourier maps and refined isotropically (except for carboxy atom H1, which was placed and fixed at its calculated position), with $U_{\rm iso}$(H) values set at 0.05 Å^2, using a riding model.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997 *PLATON* (Spek, 2003) and *ATOMS* (Dowty, 1995); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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