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Bis(benzylammonium) hexachlorotin(IV)

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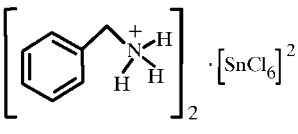
The crystal structure of bis(benzylammonium) hexachlorotin(IV), $(C_7H_7NH_3)_2[SnCl_6]$, exhibits ionic layers separated by hydrocarbon layers. The hydrocarbon layer contains two crystallographically inequivalent benzyl groups and aromatic π–π stacking interactions are observed in this layer. In the inorganic layer, the ammonium groups interact with isolated tilted $[SnCl_6]^{2-}$ octahedra through normal, bifurcated and trifurcated N—H···Cl hydrogen bonds.

Comment

Due to their two-dimensional structure and interesting magnetic and electronic properties, organic–inorganic hybrid compounds of the formula $(R\text{–}NH_3)_2SnX_4$ (where X is F, Cl, Br or I) have attracted a great deal of attention (Koutselas *et al.*, 1996; Mitzi *et al.*, 1998; Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002). On the other hand, the structural characteristics of compounds with the formula $(R\text{–}NH_3)_2SnX_6$ have not been investigated extensively. The crystal structures of only four primary *n*-alkylammonium hexachlorotin(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). No crystal structure of an arylammonium hexachlorotin(IV) compound has been reported previously. In this investigation, the crystal structure of bis(benzylammonium) hexachlorotin(IV), (I), was determined and the results are presented here.



(I)

The molecular geometry and atom-numbering scheme used are shown in Fig. 1. The structure of (I) consists of alternating ionic and hydrocarbon layers. The hydrocarbon layer is comprised of benzyl moeties, and the ionic layer contains ammonium groups and $[SnCl_6]^{2-}$ octahedra.

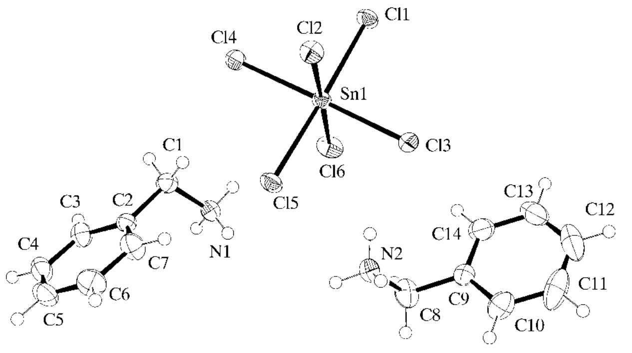


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level.

In the hydrocarbon layer, the aromatic rings are interdigitated and tilted relative to the ionic layer. There are two crystallographically inequivalent benzylammonium cations in the asymmetric unit. For the two cations, the atoms constituting each of the aromatic rings are coplanar, with r.m.s. deviations of 0.003 and 0.007 Å. The angle between the planes through the aromatic rings is 24.2 (2)°. The two aromatic ring planes are tilted by angles of 68.27 (14) and 87.98 (15)° relative to the ionic layer. Intermolecular π–π interactions are evident, with a short centroid-to-centroid distance of 3.773 (4) Å.

In the ionic layer, extending parallel to the *ab* plane, isolated distorted $[SnCl_6]^{2-}$ octahedra interact with ammonium groups *via* hydrogen bonds. Unlike the $(R\text{–}NH_3)_2SnX_4$ structures, the $[SnCl_6]^{2-}$ octahedra in (I) do not share corners.

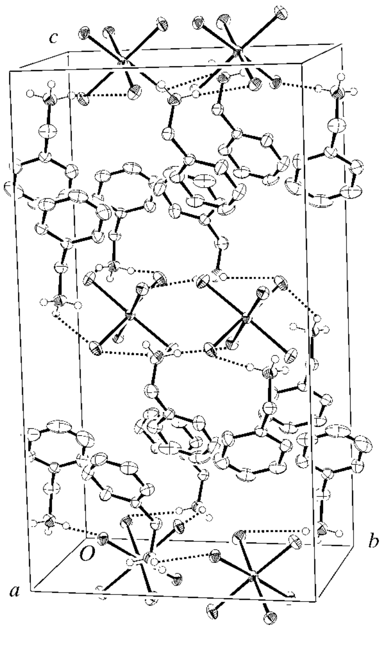


Figure 2
Packing diagram for (I), viewed down the *a* axis, showing the layered packing and interdigitation, together with some of the N—H···Cl interactions.

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The two ammonium groups in the asymmetric unit of (I) display different hydrogen-bonding interactions with Cl atoms. Atom N1 is hydrogen bonded to five Cl atoms through four bifurcated and one normal hydrogen bond. Atom N2 is also hydrogen bonded to five Cl atoms, but through two normal hydrogen bonds and one trifurcated hydrogen bond. Hydrogen-bonding donor–acceptor distances range from 3.282 (5) to 3.631 (5) Å. Sn—Cl bond lengths differ significantly (Table 1), and range from 2.1064 (14) to 2.4590 (12) Å. The Sn—Cl bond lengths for the Cl atoms engaged in strong hydrogen bonding, *i.e.* atoms Cl5 [N2(—H2*C*)···Cl5 = 3.282 (5) Å], Cl2 [N2(—H2*A*)···Cl2 = 3.357 (4) Å] and Cl6 [N1(—H1*A*)···Cl6 = 3.464 Å], are elongated. Additional hydrogen-bonding parameters are listed in Table 2. The $[SnCl_6]^{2-}$ octahedra are tilted relative to the *ab* plane by an angle of 40.06 (4)°. In consecutive ionic layers, the octahedra have opposite tilt directions. The tilted octahedra and layered packing are illustrated in Fig. 2.

Experimental

Benzylammonium chloride was prepared by the dropwise addition of concentrated hydrochloric acid (37%, Aldrich) to a solution of benzylamine (99%, Saarchem) in chloroform (99%, Saarchem). The precipitate was filtered off and allowed to dry. The title compound was crystallized by slow evaporation of a methanol solution of $SnCl_2 \cdot H_2O$ (96%, Saarchem) and benzylammonium chloride (1:2 stoichiometric ratio) at room temperature. A plate-like colourless crystal of (I) was selected for the X-ray diffraction study.

Crystal data

$(C_7H_{10}N)_2[SnCl_6]$
$M_r = 547.71$
Monoclinic, $P2_1/c$
$a = 7.612$ (2) Å
$b = 12.409$ (8) Å
$c = 22.032$ (7) Å
$\beta = 94.97$ (3)°
$V = 2073.3$ (16) Å^3
$Z = 4$
$D_x = 1.755$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 60 reflections
$\theta = 2$–32°
$\mu = 2.01$ mm^{-1}
$T = 180$ (2) K
Plate, colourless
0.60 × 0.30 × 0.15 mm

Data collection

Oxford XCALIBUR2 diffractometer
ω/φ scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.350$, $T_{\max} = 0.741$
19 081 measured reflections
6478 independent reflections
5440 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\max} = 32.0°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 18$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.120$
$S = 1.16$
6478 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 10.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.63$ e Å^{-3}
$\Delta\rho_{\min} = -0.99$ e Å^{-3}

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å and N—H distances of 0.89 Å, and were refined using a riding model, with $U_{\rm iso}(H) = 1.5U_{\rm eq}$(parent atom).

Table 1
Selected interatomic distances (Å).

Sn1—Cl5	2.4415 (12)	Sn1—Cl1	2.4242 (12)
Sn1—Cl6	2.4271 (13)	Sn1—Cl4	2.4244 (14)
Sn1—Cl3	2.4064 (14)	Sn1—Cl2	2.4590 (12)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl4$^{\rm i}$	0.89	2.78	3.494 (4)	138
N1—H1*A*···Cl6	0.89	2.80	3.464 (4)	133
N1—H1*B*···Cl4$^{\rm ii}$	0.89	2.62	3.366 (4)	143
N1—H1*B*···Cl1$^{\rm i}$	0.89	2.86	3.481 (5)	128
N1—H1*C*···Cl2$^{\rm ii}$	0.89	2.56	3.377 (4)	153
N2—H2*A*···Cl2$^{\rm ii}$	0.89	2.48	3.357 (4)	169
N2—H2*B*···Cl3	0.89	2.65	3.393 (4)	142
N2—H2*B*···Cl6	0.89	2.88	3.631 (5)	142
N2—H2*B*···Cl5	0.89	2.96	3.383 (4)	111
N2—H2*C*···Cl5$^{\rm iii}$	0.89	2.41	3.282 (5)	166

Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $1 + x, y, z$; (iii) $1 - x, 1 - y, 1 - z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DN1036). Services for accessing these data are described at the back of the journal.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Elleuch, H., Kamoun, M., Daoud, A. & Jouini, T. (1996). *Phys. Status Solidi A*, **157**, 3–9.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kagan, C. R., Mitzi, D. B. & Dimitrakopoulos, C. D. (1999). *Science*, **286**, 945–947.
Kitahama, K., Kiriyama, H. & Baba, Y. (1979). *Bull. Chem. Soc. Jpn*, **52**, 324–328.
Knop, O., Cameron, T. S., James, M. A. & Falk, M. (1983). *Can. J. Chem.* **61**, 1620–1650.
Koutselas, I. B., Ducasse, L. & Papavassiliou, G. C. (1996). *J. Phys. Condens. Matter*, **8**, 1217–1227.
Mitzi, D. B., Liang, K. & Wang, S. (1998). *Inorg. Chem.* **37**, 321–327.
Oxford Diffraction (2003). *CrysAlis CCD* and *CrysAlis RED*. Versions 1170. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Raptopoulou, C. P., Terzis, A., Mousdis, G. A. & Papavassiliou, G. C. (2002). *Z. Naturforsch. Teil B*, **57**, 645–650.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.