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Bis(benzyltriethylammonium) hexachloridostannate(IV)

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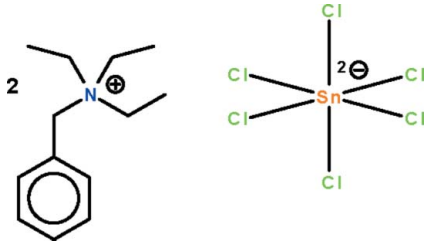
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.021; wR factor = 0.059; data-to-parameter ratio = 23.5.

The reaction between benzyltriethylammonium chloride and dimethyltin dichloride yields the title salt, $[(C_6H_5CH_2)(C_2H_5)_3N]_2[SnCl_6]$. The Sn^{IV} atom, located on a center of inversion, exists in an octahedral coordination environment. The cation links with the anion *via* weak C—H···Cl hydrogen bonding.

Related literature

For bis(tetramethylammonium) hexachloridostannate(IV), see: Furukawa *et al.* (1982). For bis(tetra-*n*-propylammonium) hexachloridostannate(IV), see: James *et al.* (1992). For bis(tetraethylammonium) hexachloridostannate(IV), see: Sowa *et al.* (1981).



Experimental

Crystal data

$(C_{13}H_{22}N)_2[SnCl_6]$
M_r = 716.02
Monoclinic, $P2_1/n$
a = 11.2096 (6) Å
b = 11.2306 (6) Å
c = 12.9796 (7) Å
β = 90.872 (1)°
V = 1633.82 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 295 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.698, T_{max} = 0.882
15028 measured reflections
3756 independent reflections
3276 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.059
S = 1.01
3756 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···Cl1^{i}	0.96	2.74	3.685 (3)	169

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5035).

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supporting information

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S1. Comment

The reaction of dimethyltin dichloride with ammonium halides sometimes leads to tin-carbon cleave to result in the formation of a hexahalogenostannate. Tin-methyl cleavage was noted in the reaction of dimethyltin dichloride with and benzyltriethylammonium chloride; the resulting the title salt (Scheme I, Fig. 1) consists of ammonium cations and hexachloridostannate anions. The reported ammonium hexachloridostannates all have symmetrically substituted ammonium cations.

S2. Experimental

Dimethyltin(IV) dichloride (0.219 g, 1 mmol) and benzyltriethylammonium chloride (0.455 g, 2 mmol) were dissolved in methanol and the solution kept at 333 K. Crystals were isolated after several days; m.p. 452–454 K.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C).

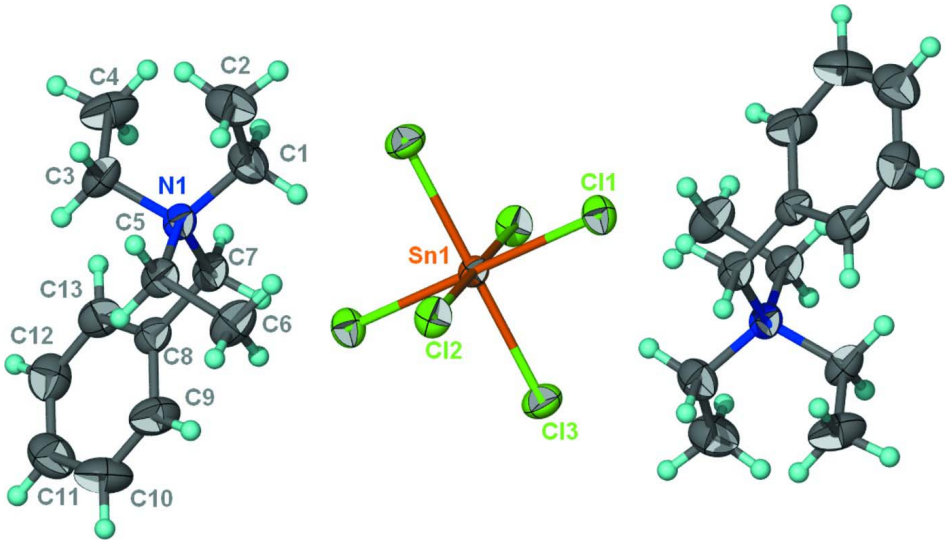

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the $2(C_6H_5CH_2)(C_2H_5)_3N^+$ $SnCl_6^{2-}$ salt at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Bis(benzyltriethylammonium) hexachloridostannate(IV)

Crystal data

$(C_{13}H_{22}N)_2[SnCl_6]$
M_r = 716.02
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.2096 (6) Å
b = 11.2306 (6) Å
c = 12.9796 (7) Å
β = 90.872 (1)°
V = 1633.82 (15) Å^3
Z = 2
$F(000)$ = 732
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8245 reflections
θ = 2.4–28.2°
μ = 1.29 mm^{-1}
T = 295 K
Prism, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.698, T_{max} = 0.882
15028 measured reflections
3756 independent reflections
3276 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −14→13
k = −14→14
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.059
S = 1.01
3756 reflections
160 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.4848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.5000	0.5000	0.5000	0.03041 (6)
Cl1	0.53546 (4)	0.67877 (4)	0.60050 (3)	0.04330 (11)
Cl2	0.45054 (4)	0.39111 (4)	0.65796 (3)	0.04483 (12)
Cl3	0.70731 (4)	0.44472 (5)	0.52383 (4)	0.04963 (13)
N1	0.10908 (13)	0.22025 (14)	0.56788 (12)	0.0390 (3)
C1	0.1030 (2)	0.3475 (2)	0.60638 (18)	0.0534 (5)
H1A	0.1762	0.3649	0.6443	0.064*
H1B	0.0997	0.4002	0.5472	0.064*
C2	−0.0015 (2)	0.3758 (2)	0.6748 (2)	0.0659 (7)
H2A	0.0027	0.4576	0.6958	0.099*
H2B	0.0013	0.3254	0.7345	0.099*
H2C	−0.0748	0.3622	0.6373	0.099*
C3	−0.00149 (17)	0.1864 (2)	0.50650 (16)	0.0519 (5)

H3A	−0.0680	0.1816	0.5533	0.062*
H3B	0.0103	0.1075	0.4779	0.062*
C4	−0.0354 (2)	0.2704 (3)	0.41919 (19)	0.0744 (8)
H4A	−0.1066	0.2421	0.3853	0.112*
H4B	0.0283	0.2736	0.3707	0.112*
H4C	−0.0492	0.3486	0.4464	0.112*
C5	0.11816 (18)	0.13332 (19)	0.65726 (15)	0.0460 (5)
H5A	0.1295	0.0539	0.6296	0.055*
H5B	0.0429	0.1336	0.6932	0.055*
C6	0.2178 (2)	0.1584 (3)	0.73500 (17)	0.0627 (6)
H6A	0.2181	0.0979	0.7873	0.094*
H6B	0.2051	0.2348	0.7662	0.094*
H6C	0.2930	0.1583	0.7007	0.094*
C7	0.22048 (17)	0.21310 (18)	0.50080 (15)	0.0436 (4)
H7A	0.2122	0.2710	0.4457	0.052*
H7B	0.2891	0.2363	0.5426	0.052*
C8	0.24596 (17)	0.09404 (19)	0.45360 (15)	0.0429 (4)
C9	0.3185 (3)	0.0112 (2)	0.5036 (2)	0.0660 (7)
H9	0.3492	0.0284	0.5689	0.079*
C10	0.3458 (3)	−0.0965 (3)	0.4577 (2)	0.0798 (8)
H10	0.3933	−0.1515	0.4927	0.096*
C11	0.3032 (3)	−0.1225 (2)	0.3612 (2)	0.0713 (7)
H11	0.3217	−0.1949	0.3306	0.086*
C12	0.2334 (2)	−0.0415 (3)	0.3098 (2)	0.0632 (6)
H12	0.2049	−0.0587	0.2438	0.076*
C13	0.2049 (2)	0.0659 (2)	0.35541 (16)	0.0524 (5)
H13	0.1574	0.1202	0.3195	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02733 (9)	0.03422 (10)	0.02977 (9)	−0.00209 (6)	0.00331 (6)	0.00222 (6)
Cl1	0.0462 (3)	0.0419 (2)	0.0420 (2)	−0.0050 (2)	0.00723 (19)	−0.00544 (19)
Cl2	0.0483 (3)	0.0508 (3)	0.0354 (2)	−0.0082 (2)	0.00231 (18)	0.00960 (19)
Cl3	0.0344 (2)	0.0550 (3)	0.0595 (3)	0.0041 (2)	0.0010 (2)	0.0053 (2)
N1	0.0344 (8)	0.0408 (8)	0.0418 (8)	−0.0066 (6)	0.0041 (6)	0.0081 (7)
C1	0.0606 (14)	0.0438 (11)	0.0561 (12)	−0.0041 (10)	0.0122 (10)	0.0042 (9)
C2	0.0721 (16)	0.0610 (15)	0.0650 (15)	0.0120 (13)	0.0182 (12)	0.0052 (12)
C3	0.0346 (10)	0.0675 (15)	0.0536 (12)	−0.0047 (9)	−0.0041 (9)	0.0039 (10)
C4	0.0640 (16)	0.101 (2)	0.0578 (14)	0.0305 (15)	−0.0091 (12)	0.0077 (14)
C5	0.0429 (11)	0.0497 (11)	0.0454 (10)	−0.0070 (9)	0.0037 (8)	0.0154 (9)
C6	0.0511 (13)	0.0902 (19)	0.0467 (12)	−0.0049 (12)	−0.0053 (10)	0.0124 (12)
C7	0.0375 (10)	0.0483 (11)	0.0453 (10)	−0.0073 (8)	0.0074 (8)	0.0075 (8)
C8	0.0348 (10)	0.0498 (11)	0.0443 (10)	−0.0025 (8)	0.0033 (8)	0.0071 (8)
C9	0.0628 (16)	0.0793 (19)	0.0554 (14)	0.0197 (13)	−0.0120 (12)	0.0016 (12)
C10	0.081 (2)	0.0746 (19)	0.084 (2)	0.0352 (16)	−0.0011 (15)	0.0087 (15)
C11	0.0777 (18)	0.0575 (15)	0.0793 (18)	0.0054 (13)	0.0182 (14)	−0.0086 (13)
C12	0.0640 (15)	0.0723 (16)	0.0535 (13)	−0.0050 (13)	0.0044 (11)	−0.0103 (12)

C13	0.0502 (12)	0.0615 (14)	0.0453 (11)	0.0037 (10)	−0.0008 (9)	0.0070 (10)

Geometric parameters (Å, º)

Sn1—Cl3^{i}	2.4207 (5)	C4—H4C	0.9600
Sn1—Cl3	2.4207 (5)	C5—C6	1.520 (3)
Sn1—Cl1	2.4237 (5)	C5—H5A	0.9700
Sn1—Cl1^{i}	2.4237 (5)	C5—H5B	0.9700
Sn1—Cl2^{i}	2.4579 (4)	C6—H6A	0.9600
Sn1—Cl2	2.4579 (4)	C6—H6B	0.9600
N1—C3	1.512 (2)	C6—H6C	0.9600
N1—C1	1.515 (3)	C7—C8	1.500 (3)
N1—C5	1.518 (2)	C7—H7A	0.9700
N1—C7	1.535 (2)	C7—H7B	0.9700
C1—C2	1.515 (3)	C8—C13	1.385 (3)
C1—H1A	0.9700	C8—C9	1.390 (3)
C1—H1B	0.9700	C9—C10	1.386 (4)
C2—H2A	0.9600	C9—H9	0.9300
C2—H2B	0.9600	C10—C11	1.364 (4)
C2—H2C	0.9600	C10—H10	0.9300
C3—C4	1.519 (3)	C11—C12	1.367 (4)
C3—H3A	0.9700	C11—H11	0.9300
C3—H3B	0.9700	C12—C13	1.384 (4)
C4—H4A	0.9600	C12—H12	0.9300
C4—H4B	0.9600	C13—H13	0.9300
Cl3^{i}—Sn1—Cl3	180.0	H4A—C4—H4B	109.5
Cl3^{i}—Sn1—Cl1	90.320 (18)	C3—C4—H4C	109.5
Cl3—Sn1—Cl1	89.680 (18)	H4A—C4—H4C	109.5
Cl3^{i}—Sn1—Cl1^{i}	89.680 (18)	H4B—C4—H4C	109.5
Cl3—Sn1—Cl1^{i}	90.320 (18)	N1—C5—C6	115.36 (17)
Cl1—Sn1—Cl1^{i}	180.0	N1—C5—H5A	108.4
Cl3^{i}—Sn1—Cl2^{i}	89.662 (17)	C6—C5—H5A	108.4
Cl3—Sn1—Cl2^{i}	90.338 (17)	N1—C5—H5B	108.4
Cl1—Sn1—Cl2^{i}	89.974 (17)	C6—C5—H5B	108.4
Cl1^{i}—Sn1—Cl2^{i}	90.026 (17)	H5A—C5—H5B	107.5
Cl3^{i}—Sn1—Cl2	90.338 (17)	C5—C6—H6A	109.5
Cl3—Sn1—Cl2	89.662 (17)	C5—C6—H6B	109.5
Cl1—Sn1—Cl2	90.026 (17)	H6A—C6—H6B	109.5
Cl1^{i}—Sn1—Cl2	89.974 (17)	C5—C6—H6C	109.5
Cl2^{i}—Sn1—Cl2	180.00 (2)	H6A—C6—H6C	109.5
C3—N1—C1	111.75 (17)	H6B—C6—H6C	109.5
C3—N1—C5	106.60 (15)	C8—C7—N1	116.09 (15)
C1—N1—C5	110.92 (16)	C8—C7—H7A	108.3
C3—N1—C7	110.82 (15)	N1—C7—H7A	108.3
C1—N1—C7	106.10 (14)	C8—C7—H7B	108.3
C5—N1—C7	110.73 (15)	N1—C7—H7B	108.3
C2—C1—N1	115.49 (18)	H7A—C7—H7B	107.4

C2—C1—H1A	108.4	C13—C8—C9	117.5 (2)
N1—C1—H1A	108.4	C13—C8—C7	121.09 (19)
C2—C1—H1B	108.4	C9—C8—C7	121.3 (2)
N1—C1—H1B	108.4	C10—C9—C8	121.0 (2)
H1A—C1—H1B	107.5	C10—C9—H9	119.5
C1—C2—H2A	109.5	C8—C9—H9	119.5
C1—C2—H2B	109.5	C11—C10—C9	120.3 (3)
H2A—C2—H2B	109.5	C11—C10—H10	119.8
C1—C2—H2C	109.5	C9—C10—H10	119.8
H2A—C2—H2C	109.5	C10—C11—C12	119.7 (3)
H2B—C2—H2C	109.5	C10—C11—H11	120.1
N1—C3—C4	115.5 (2)	C12—C11—H11	120.1
N1—C3—H3A	108.4	C11—C12—C13	120.4 (2)
C4—C3—H3A	108.4	C11—C12—H12	119.8
N1—C3—H3B	108.4	C13—C12—H12	119.8
C4—C3—H3B	108.4	C8—C13—C12	121.1 (2)
H3A—C3—H3B	107.5	C8—C13—H13	119.4
C3—C4—H4A	109.5	C12—C13—H13	119.4
C3—C4—H4B	109.5		

C3—N1—C1—C2	58.9 (2)	C5—N1—C7—C8	59.4 (2)
C5—N1—C1—C2	−59.9 (2)	N1—C7—C8—C13	93.4 (2)
C7—N1—C1—C2	179.8 (2)	N1—C7—C8—C9	−91.3 (3)
C1—N1—C3—C4	52.4 (2)	C13—C8—C9—C10	−1.7 (4)
C5—N1—C3—C4	173.76 (19)	C7—C8—C9—C10	−177.2 (3)
C7—N1—C3—C4	−65.7 (2)	C8—C9—C10—C11	1.1 (5)
C3—N1—C5—C6	−174.68 (19)	C9—C10—C11—C12	0.0 (5)
C1—N1—C5—C6	−52.8 (2)	C10—C11—C12—C13	−0.5 (4)
C7—N1—C5—C6	64.7 (2)	C9—C8—C13—C12	1.2 (3)
C3—N1—C7—C8	−58.7 (2)	C7—C8—C13—C12	176.7 (2)
C1—N1—C7—C8	179.82 (17)	C11—C12—C13—C8	−0.1 (4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···Cl1^{ii}	0.96	2.74	3.685 (3)	169

Symmetry code: (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.