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Bis(4-acetylanilinium) hexachloridostannate(IV)

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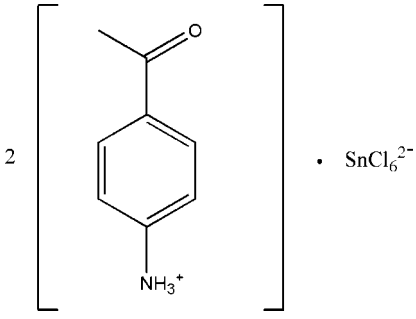
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 15.8.

In the title compound, $(C_8H_{10}NO)_2[SnCl_6]$, the Sn^{IV} atom exists in an octahedral coordination environment. In the crystal, intermolecular N—H···O and N—H···Cl hydrogen bonds link the cations and anions into a three-dimensional framework.

Related literature

For general background to inorganic–organic hybrid compounds, see: Antonietti & Ozin (2004); Cong & Yu (2009); Descazo *et al.* (2006); Li *et al.* (2007); Sanchez *et al.* (2005).



Experimental

Crystal data

$(C_8H_{10}NO)_2[SnCl_6]$
M_r = 603.73
Monoclinic, $P2_1/c$
a = 7.2540 (8) Å
b = 12.6481 (13) Å
c = 24.438 (2) Å
β = 93.991 (1)°
V = 2236.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.87 mm^{-1}
T = 298 K
0.48 × 0.44 × 0.43 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.467, T_{max} = 0.500
10422 measured reflections
3929 independent reflections
2996 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 1.00
3929 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.89	2.06	2.939 (7)	170
N1—H1B···O2^{ii}	0.89	2.01	2.884 (6)	168
N1—H1A···Cl1^{iii}	0.89	2.49	3.322 (6)	156
N2—H2B···Cl2^{i}	0.89	2.59	3.350 (6)	144
N2—H2C···Cl3^{iv}	0.89	2.69	3.321 (5)	129
N1—H1C···Cl5^{v}	0.89	2.55	3.367 (5)	153
N2—H2C···Cl6^{iv}	0.89	2.64	3.442 (5)	151

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5184).

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supporting information

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Bis(4-acetylanilinium) hexachloridostannate(IV)

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S1. Comment

Inorganic-organic hybrid materials have received much attention due to their potential applications in many areas such as gas storage, separation, catalysis, magnetism, optics as well as in electrical conductivity (Descazo *et al.*, 2006; Li *et al.*, 2007; Sanchez *et al.*, 2005). Recently, we have prepared the title compound and here its crystal structure is reported.

This title compound contains $SnC1_6$ inorganic anions and organic cations. The $SnCl_6$ inorganic anion adopts a regular octahedral geometry, with average Sn—Cl distance of 2.4102 Å. In the organic cations, the diangle between the methyl ketone and the phenyl ring is 14.9 (3)° or 3.1 (2)°.

In the crystal structure, intermolecular N—H···O and N—H···Cl hydrogen bonds link cations and anions into a three-dimensioal framework.

S2. Experimental

p-Aminoacetophenone (10 mmol) was dissolved in methanol (10 ml). Ten minutes later, a methanol solution (10 ml) of tin tetrachloride (5 mmol) was added with stirring. The reaction mixture was stirred for 4 h. The solution was held at room temperature for about two weeks, whereupon yellow crystals suitable for X-ray diffraction analysis were obtained.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model, with C–H = 0.96 Å (methyl), 0.93 Å (aromatic), N–H = 0.89 Å (ammonium) and U_{iso}(H) = 1.5U_{eq}(C_{methyl},N) and 1.2U_{eq}(C).

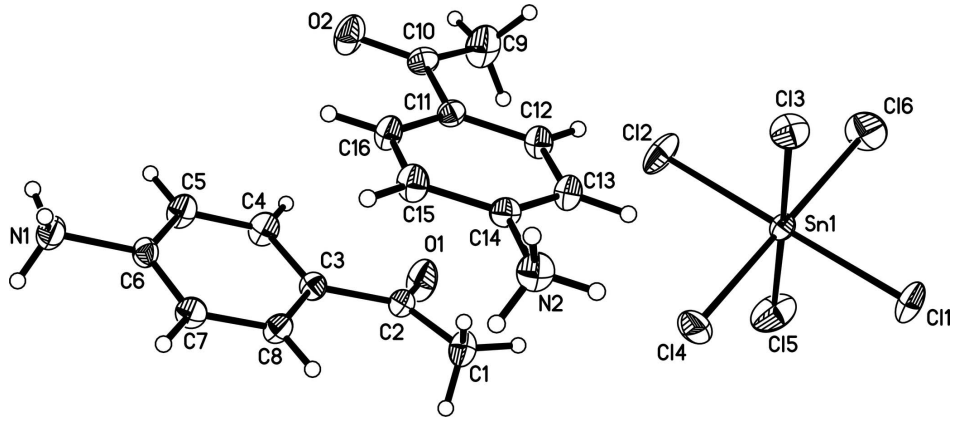

Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Bis(4-acetylanilinium) hexachloridostannate(IV)

Crystal data

$(C_8H_{10}NO)_2[SnCl_6]$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.2540$ (8) Å
$b = 12.6481$ (13) Å
$c = 24.438$ (2) Å
$\beta = 93.991$ (1)°
$V = 2236.7$ (4) Å^3
$Z = 4$
$F(000) = 1192$
$D_x = 1.793$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3529 reflections
$\theta = 2.5$–$27.3°$
$\mu = 1.87$ mm^{-1}
$T = 298$ K
Block, yellow
0.48 × 0.44 × 0.43 mm

Data collection

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Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.467$, $T_{max} = 0.500$
10422 measured reflections
3929 independent reflections
2996 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -8 \rightarrow 8$
$k = -15 \rightarrow 14$
$l = -23 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.112$
$S = 1.00$
3929 reflections
248 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
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 4.9089P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -0.83$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.26788 (5)	0.33553 (3)	0.392680 (15)	0.02996 (14)
Cl1	0.2381 (3)	0.19836 (12)	0.46029 (6)	0.0541 (5)
Cl2	0.2941 (3)	0.47370 (13)	0.32429 (7)	0.0631 (5)
Cl3	0.0010 (2)	0.26670 (12)	0.33926 (7)	0.0492 (4)

Cl4	0.4656 (3)	0.22042 (16)	0.34441 (7)	0.0645 (5)
Cl5	0.5344 (3)	0.40331 (15)	0.44385 (9)	0.0763 (6)
Cl6	0.0643 (3)	0.44692 (15)	0.43985 (8)	0.0706 (6)
N1	0.7808 (7)	0.3221 (4)	−0.04410 (19)	0.0425 (12)
H1A	0.8949	0.3038	−0.0516	0.064*
H1B	0.7532	0.3847	−0.0591	0.064*
H1C	0.7011	0.2739	−0.0578	0.064*
N2	0.2441 (7)	−0.0116 (4)	0.1716 (2)	0.0435 (13)
H2A	0.2336	−0.0262	0.2069	0.065*
H2B	0.3501	−0.0378	0.1612	0.065*
H2C	0.1501	−0.0406	0.1515	0.065*
O1	0.7432 (7)	0.4341 (3)	0.21126 (18)	0.0580 (13)
O2	0.2530 (7)	0.4680 (3)	0.08980 (18)	0.0539 (12)
C1	0.7034 (9)	0.2499 (5)	0.2194 (2)	0.0438 (15)
H1D	0.6742	0.2672	0.2560	0.066*
H1E	0.8139	0.2079	0.2207	0.066*
H1F	0.6032	0.2106	0.2015	0.066*
C2	0.7326 (8)	0.3483 (5)	0.1884 (2)	0.0367 (14)
C3	0.7471 (8)	0.3413 (4)	0.1275 (2)	0.0311 (12)
C4	0.7306 (9)	0.4318 (4)	0.0953 (2)	0.0418 (15)
H4	0.7124	0.4969	0.1117	0.050*
C5	0.7409 (9)	0.4261 (4)	0.0395 (2)	0.0409 (15)
H5	0.7288	0.4865	0.0179	0.049*
C6	0.7697 (8)	0.3287 (4)	0.0163 (2)	0.0323 (13)
C7	0.7890 (8)	0.2386 (4)	0.0465 (2)	0.0357 (14)
H7	0.8114	0.1742	0.0298	0.043*
C8	0.7747 (8)	0.2445 (4)	0.1024 (2)	0.0352 (13)
H8	0.7836	0.1833	0.1235	0.042*
C9	0.2098 (11)	0.5103 (5)	0.1816 (3)	0.060 (2)
H9A	0.2172	0.5817	0.1685	0.091*
H9B	0.3052	0.4986	0.2102	0.091*
H9C	0.0912	0.4990	0.1957	0.091*
C10	0.2339 (8)	0.4365 (4)	0.1361 (3)	0.0367 (14)
C11	0.2402 (7)	0.3190 (4)	0.1471 (2)	0.0291 (12)
C12	0.2097 (8)	0.2773 (4)	0.1983 (2)	0.0334 (13)
H12	0.1874	0.3226	0.2271	0.040*
C13	0.2122 (8)	0.1688 (4)	0.2070 (2)	0.0361 (13)
H13	0.1942	0.1407	0.2414	0.043*
C14	0.2417 (7)	0.1046 (4)	0.1635 (2)	0.0309 (13)
C15	0.2731 (9)	0.1431 (4)	0.1123 (2)	0.0393 (15)
H15	0.2941	0.0973	0.0836	0.047*
C16	0.2725 (8)	0.2515 (4)	0.1044 (2)	0.0368 (14)
H16	0.2939	0.2790	0.0701	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0358 (2)	0.0256 (2)	0.0283 (2)	−0.00138 (17)	0.00080 (15)	0.00247 (16)

Cl1	0.0862 (13)	0.0402 (9)	0.0365 (9)	−0.0050 (8)	0.0079 (8)	0.0140 (7)
Cl2	0.0919 (14)	0.0452 (10)	0.0497 (10)	−0.0193 (9)	−0.0122 (9)	0.0256 (8)
Cl3	0.0447 (9)	0.0490 (9)	0.0523 (10)	−0.0104 (7)	−0.0098 (8)	−0.0073 (7)
Cl4	0.0585 (12)	0.0893 (14)	0.0474 (10)	0.0312 (10)	0.0165 (8)	−0.0046 (9)
Cl5	0.0737 (14)	0.0646 (12)	0.0854 (15)	−0.0219 (10)	−0.0323 (11)	0.0147 (10)
Cl6	0.0885 (15)	0.0613 (11)	0.0630 (12)	0.0274 (10)	0.0125 (11)	−0.0232 (9)
N1	0.056 (3)	0.042 (3)	0.030 (3)	0.005 (2)	0.003 (2)	0.001 (2)
N2	0.054 (3)	0.028 (3)	0.049 (3)	−0.003 (2)	0.006 (3)	−0.002 (2)
O1	0.100 (4)	0.038 (3)	0.036 (3)	−0.001 (2)	0.012 (2)	−0.010 (2)
O2	0.086 (4)	0.035 (2)	0.042 (3)	0.006 (2)	0.013 (2)	0.012 (2)
C1	0.051 (4)	0.050 (4)	0.031 (3)	−0.007 (3)	0.005 (3)	0.001 (3)
C2	0.036 (3)	0.045 (4)	0.029 (3)	0.005 (3)	0.002 (3)	0.003 (3)
C3	0.033 (3)	0.032 (3)	0.028 (3)	−0.002 (2)	−0.001 (2)	−0.005 (2)
C4	0.066 (4)	0.021 (3)	0.038 (4)	0.005 (3)	0.005 (3)	−0.006 (2)
C5	0.063 (4)	0.024 (3)	0.036 (3)	0.001 (3)	0.004 (3)	0.000 (2)
C6	0.037 (3)	0.034 (3)	0.025 (3)	0.000 (3)	0.003 (2)	−0.005 (2)
C7	0.048 (4)	0.021 (3)	0.038 (3)	0.003 (2)	0.004 (3)	−0.004 (2)
C8	0.043 (4)	0.033 (3)	0.029 (3)	0.001 (3)	−0.002 (3)	0.001 (2)
C9	0.097 (6)	0.025 (3)	0.061 (5)	0.004 (3)	0.018 (4)	0.006 (3)
C10	0.039 (4)	0.030 (3)	0.040 (4)	0.005 (3)	0.001 (3)	0.004 (3)
C11	0.030 (3)	0.027 (3)	0.030 (3)	−0.001 (2)	0.000 (2)	0.001 (2)
C12	0.042 (3)	0.027 (3)	0.032 (3)	−0.002 (2)	0.006 (3)	−0.004 (2)
C13	0.044 (4)	0.034 (3)	0.031 (3)	−0.006 (3)	0.006 (3)	0.001 (3)
C14	0.030 (3)	0.025 (3)	0.038 (3)	−0.003 (2)	0.002 (3)	0.003 (2)
C15	0.053 (4)	0.031 (3)	0.035 (3)	−0.002 (3)	0.007 (3)	−0.009 (2)
C16	0.049 (4)	0.033 (3)	0.029 (3)	−0.001 (3)	0.006 (3)	0.003 (2)

Geometric parameters (Å, º)

Sn1—Cl5	2.3873 (18)	C4—C5	1.373 (8)
Sn1—Cl6	2.3938 (17)	C4—H4	0.93
Sn1—Cl4	2.4090 (17)	C5—C6	1.378 (7)
Sn1—Cl1	2.4158 (15)	C5—H5	0.93
Sn1—Cl3	2.4206 (15)	C6—C7	1.360 (7)
Sn1—Cl2	2.4346 (15)	C7—C8	1.379 (8)
N1—C6	1.486 (7)	C7—H7	0.93
N1—H1A	0.89	C8—H8	0.93
N1—H1B	0.89	C9—C10	1.471 (9)
N1—H1C	0.89	C9—H9A	0.96
N2—C14	1.482 (7)	C9—H9B	0.96
N2—H2A	0.89	C9—H9C	0.96
N2—H2B	0.89	C10—C11	1.509 (7)
N2—H2C	0.89	C11—C16	1.381 (8)
O1—C2	1.220 (7)	C11—C12	1.390 (8)
O2—C10	1.217 (7)	C12—C13	1.389 (7)
C1—C2	1.480 (8)	C12—H12	0.93
C1—H1D	0.96	C13—C14	1.365 (8)
C1—H1E	0.96	C13—H13	0.93

C1—H1F	0.96	C14—C15	1.378 (8)
C2—C3	1.502 (8)	C15—C16	1.384 (8)
C3—C4	1.389 (8)	C15—H15	0.93
C3—C8	1.390 (7)	C16—H16	0.93
Cl5—Sn1—Cl6	92.32 (8)	C3—C4—H4	119.6
Cl5—Sn1—Cl4	89.17 (8)	C4—C5—C6	118.4 (5)
Cl6—Sn1—Cl4	178.43 (8)	C4—C5—H5	120.8
Cl5—Sn1—Cl1	90.42 (7)	C6—C5—H5	120.8
Cl6—Sn1—Cl1	90.34 (7)	C7—C6—C5	122.5 (5)
Cl4—Sn1—Cl1	89.16 (7)	C7—C6—N1	118.8 (5)
Cl5—Sn1—Cl3	178.91 (8)	C5—C6—N1	118.6 (5)
Cl6—Sn1—Cl3	88.53 (7)	C6—C7—C8	118.7 (5)
Cl4—Sn1—Cl3	89.98 (7)	C6—C7—H7	120.6
Cl1—Sn1—Cl3	90.25 (6)	C8—C7—H7	120.6
Cl5—Sn1—Cl2	90.16 (7)	C7—C8—C3	120.5 (5)
Cl6—Sn1—Cl2	89.33 (7)	C7—C8—H8	119.7
Cl4—Sn1—Cl2	91.16 (7)	C3—C8—H8	119.7
Cl1—Sn1—Cl2	179.35 (7)	C10—C9—H9A	109.5
Cl3—Sn1—Cl2	89.18 (6)	C10—C9—H9B	109.5
C6—N1—H1A	109.5	H9A—C9—H9B	109.5
C6—N1—H1B	109.5	C10—C9—H9C	109.5
H1A—N1—H1B	109.5	H9A—C9—H9C	109.5
C6—N1—H1C	109.5	H9B—C9—H9C	109.5
H1A—N1—H1C	109.5	O2—C10—C9	121.4 (5)
H1B—N1—H1C	109.5	O2—C10—C11	118.9 (5)
C14—N2—H2A	109.5	C9—C10—C11	119.7 (5)
C14—N2—H2B	109.5	C16—C11—C12	119.4 (5)
H2A—N2—H2B	109.5	C16—C11—C10	118.7 (5)
C14—N2—H2C	109.5	C12—C11—C10	121.9 (5)
H2A—N2—H2C	109.5	C13—C12—C11	120.8 (5)
H2B—N2—H2C	109.5	C13—C12—H12	119.6
C2—C1—H1D	109.5	C11—C12—H12	119.6
C2—C1—H1E	109.5	C14—C13—C12	118.1 (5)
H1D—C1—H1E	109.5	C14—C13—H13	121.0
C2—C1—H1F	109.5	C12—C13—H13	121.0
H1D—C1—H1F	109.5	C13—C14—C15	122.8 (5)
H1E—C1—H1F	109.5	C13—C14—N2	119.2 (5)
O1—C2—C1	121.4 (5)	C15—C14—N2	118.0 (5)
O1—C2—C3	120.0 (5)	C14—C15—C16	118.5 (5)
C1—C2—C3	118.6 (5)	C14—C15—H15	120.7
C4—C3—C8	119.0 (5)	C16—C15—H15	120.7
C4—C3—C2	120.3 (5)	C11—C16—C15	120.5 (5)
C8—C3—C2	120.8 (5)	C11—C16—H16	119.8
C5—C4—C3	120.7 (5)	C15—C16—H16	119.8
C5—C4—H4	119.6		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.89	2.06	2.939 (7)	170
N1—H1*B*···O2^{ii}	0.89	2.01	2.884 (6)	168
N1—H1*A*···Cl1^{iii}	0.89	2.49	3.322 (6)	156
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N2—H2*C*···Cl3^{iv}	0.89	2.69	3.321 (5)	129
N1—H1*C*···Cl5^{v}	0.89	2.55	3.367 (5)	153
N2—H2*C*···Cl6^{iv}	0.89	2.64	3.442 (5)	151

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*+1, −*y*+1/2, *z*−1/2; (iv) −*x*, *y*−1/2, −*z*+1/2; (v) *x*, −*y*+1/2, *z*−1/2.