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Tris(2-hydroxyanilinium) hexachlorostannate(IV) chloride trihydrate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.106
Data-to-parameter ratio = 19.5

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

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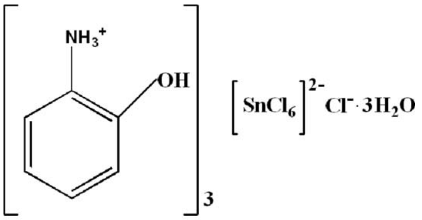
In the title compound, $(C_6H_8NO)_3[SnCl_6]Cl\cdot 3H_2O$, the asymmetric unit contains three independent cations of protonated *o*-aminophenol, one hexachlorostannate(IV) and one chloride anion, and three molecules of water. The crystal structure can be described as double layers of $[SnCl_6]$ octahedra and 2-hydroxyanilinium cations parallel to the $(10\bar{1})$ plane, with the chloride ions and the water molecules sandwiched between the double layers. A myriad of hydrogen bonds, namely, cation–cation, cation–anion, cation–water and water–water, result in a complex network of intermolecular bonds reinforcing the cohesion of the ionic structure.

Comment

Organic–inorganic hybrid materials of formula (R—NH_3), SnX_n, where X = F, Cl, Br or I, exhibit interesting magnetic, optical and electronic properties (Aruta *et al.*, 2005; Knutson & Martin, 2005; Mitzi *et al.*, 2001, Kagan *et al.*, 1999). Within our research of hybrid compounds based on tin (Bouacida *et al.*, 2005*a*,*b*,*c*), a new crystal structure has been investigated.



(I)

The asymmetric unit of the title compound, (I) (Fig. 1), contains three independent molecules of protonated *o*-aminophenol, one chloride ion, one hexachlorostannate(IV) ion and three independent water molecules. The Sn^{IV} atom is sixfold coordinated by chloride ions, forming a quasi-regular octahedral arrangement. The organic cation has the amino group protonated and takes part, together with the $[SnCl_6]^{2-}$ anions, in the formation of double layers parallel to the $(10\bar{1})$ plane (Fig. 2). The chloride ions and water molecules are sandwiched between the double layers (Fig. 2).

In this structure, four types of hydrogen bonds are observed, *viz*. cation–cation, cation–anion, cation–water and water–water, with the N and O atoms of the cation and the water molecules acting as donors and with the Cl^- ions and the O atoms of the water molecules acting as acceptors (Table 2, Fig. 3). These intermolecular bonds link the molecules within the layers and also link the layers together, forming a complex network and reinforcing the cohesion of the structure.

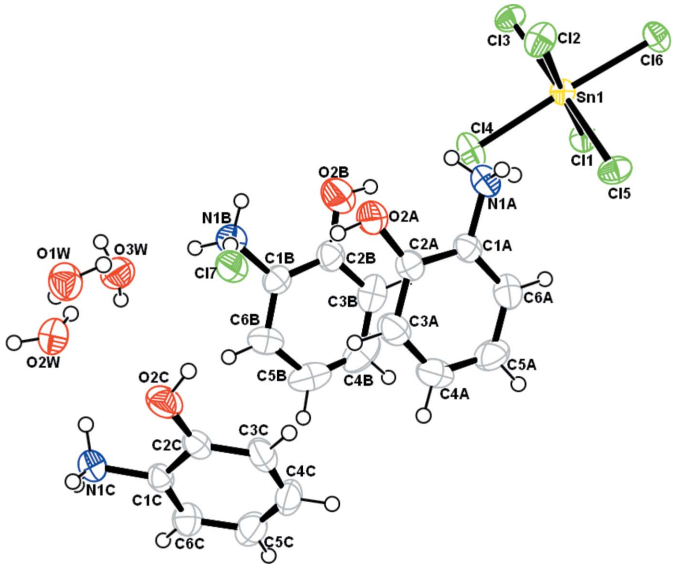


Figure 1
The structure of the title compound with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

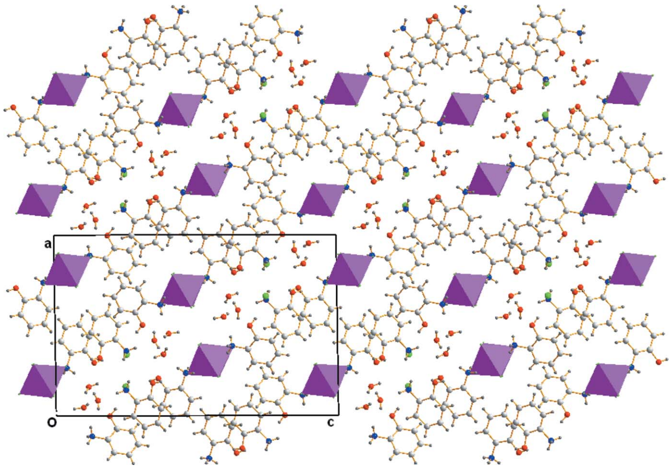


Figure 2
A diagram of the layered crystal packing in (I), viewed down the *b* axis.

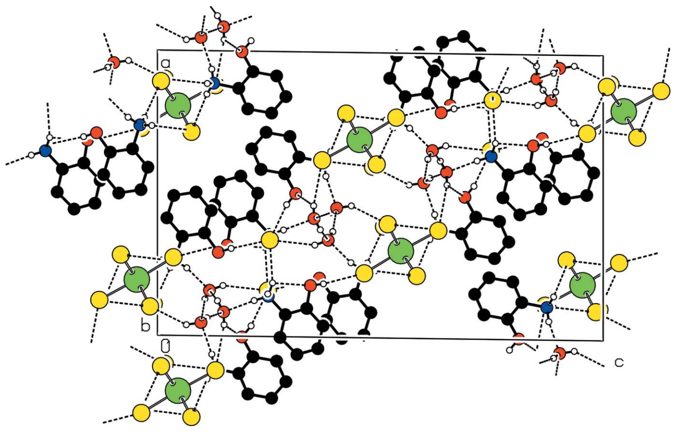


Figure 3
A view of the ionic stacking, showing the three-dimensional network of hydrogen bonds as dashed lines. H atoms not involved in hydrogen-bonding have been omitted for clarity.

Experimental

A mixture of tin(II) chloride dihydrate (50 mg, 0.2219 mmol), *o*-aminophenol (75 mg, 0.6872 mmol) and hydrochloric acid (1 ml-37%, 32.63 mmol) was added to 12 ml of distilled water in a stainless steel autoclave, with a Teflon liner, of 23 ml capacity. The autoclave was heated to 343 K and kept at this temperature for three days. Brown needle-shaped transparent crystals were obtained.

Crystal data

$(C_6H_8NO)_3[SnCl_6]Cl\cdot3H_2O$
$M_r = 751.29$
Monoclinic, $P2_1/n$
$a = 16.2653\ (2)$ Å
$b = 7.1079\ (1)$ Å
$c = 25.4562\ (5)$ Å
$\beta = 90.751\ (1)^\circ$
$V = 2942.79\ (8)$ Å^3

$Z = 4$
$D_x = 1.696$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.54$ mm^{-1}
$T = 296\ (2)$ K
Needle, brown
0.31 × 0.02 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: none
20517 measured reflections

6647 independent reflections
5218 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.106$
$S = 1.13$
6647 reflections
341 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 1.3984P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.010$
$\Delta\rho_{\max} = 1.01$ e Å^{-3}
$\Delta\rho_{\min} = -0.77$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0021 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2A—H2A···Cl7$^{\rm i}$	0.82	2.32	3.136 (3)	171
O2B—H2B···Cl4$^{\rm ii}$	0.82	2.48	3.289 (4)	168
O2C—H2C···Cl7$^{\rm i}$	0.82	2.31	3.097 (3)	162
N1A—H11A···O1W	0.89	1.94	2.816 (5)	168
N1B—H11B···Cl7$^{\rm i}$	0.89	2.33	3.214 (4)	176
N1C—H11C···Cl1$^{\rm iii}$	0.89	2.68	3.555 (3)	170
N1A—H12A···Cl5$^{\rm ii}$	0.89	2.71	3.586 (4)	167
N1B—H12B···O3$W^{\rm iv}$	0.89	1.92	2.809 (5)	174
N1C—H12C···O2$W^{\rm i}$	0.89	1.99	2.864 (5)	167
N1A—H13A···Cl3$^{\rm v}$	0.89	2.54	3.333 (4)	149
N1B—H13B···Cl7	0.89	2.46	3.227 (3)	145
N1B—H13B···O2B	0.89	2.28	2.719 (5)	110
N1C—H13C···Cl2$^{\rm vi}$	0.89	2.65	3.351 (4)	137
O1W—H12···O2W	0.86 (3)	2.04 (3)	2.881 (5)	168 (4)
O1W—H11···Cl7	0.83 (3)	2.64 (3)	3.408 (3)	155 (4)
O2W—H21···Cl2$^{\rm ii}$	0.85 (3)	2.71 (4)	3.342 (3)	133 (4)
O2W—H22···O3$W^{\rm vii}$	0.83 (4)	2.08 (4)	2.897 (5)	170 (5)
O3W—H31···O1W	0.81 (4)	2.22 (4)	2.843 (5)	135 (4)
O3W—H32···Cl6$^{\rm viii}$	0.82 (3)	2.67 (3)	3.362 (3)	144 (4)
O3W—H32···O2$C^{\rm iv}$	0.82 (3)	2.47 (4)	3.067 (5)	131 (3)

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

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H atoms of water molecules were located in difference Fourier maps and refined isotropically. All other H atoms were located in Fourier maps but introduced in calculated positions and treated as riding on their parent C, N and O atoms, with C—H distances of 0.93 Å, N—H distances of 0.89 Å and O—H distances of 0.82 Å, and with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(N,O) or 1.2$U_{\rm eq}$(C). The highest residual density peak is located 1.84 Å from atom H11*C*.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); 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) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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