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Bis(adeninium) hexachlorostannate(IV) dichloride tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.061
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.

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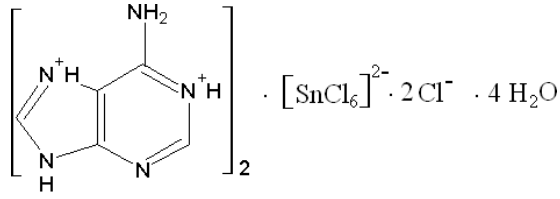
The structure of the title compound, $(C_5H_7N_5)_2[SnCl_6]Cl_2\cdot 4H_2O$, can be described as alternating layers of $C_5H_7N_5^{2+}$ and $[SnCl_6]^{2-}$ ions along the b axis, the Sn^{IV} atom lying on a twofold axis. The chloride ions are located between the organic entities, forming hydrogen bonds with the N atoms and water molecules. Layers of adeninium cations and hexachlorostannate anions are linked by anion–cation, cation–water and water–water hydrogen bonds. This three-dimensional complex network of hydrogen bonds ensures the cohesion of the ionic structure.

Comment

Studies of organic–inorganic hybrid materials have received great attention in recent years, because of their ionic, electrical, magnetic and optical properties (Hill, 1998; Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002). Adenine is one of the precursors of DNA and RNA nucleotides, and the adeninium cation (1+ or 2+) is known to form a variety of inorganic salts, such as chloride (Kistenmacher & Shigematsu, 1974), bromide (Langer & Huml, 1978*a*), bistriiodide (Cheng *et al.*, 2002), sulfate (Langer & Huml, 1978*b*), phosphate (Langer *et al.*, 1979) and nitrate (Hingerty *et al.*, 1981; Bendjeddou *et al.*, 2003; Zeleňák *et al.*, 2004).



(I)

In the present study, we present a new organic–inorganic hybrid compound, (I), based on tin and adenine, and examine the hydrogen bonding in the crystal structure.

The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1. Two imino groups of the adenine base are protoned at N1 and N7, as reported previously for the sulfate and dinitrate. The internal angles at N1 and N7 [C6—N1—C2 = 123.8 (2)° and C8—N7—C5 = 107.4 (2)°] have increased from the values of 119.8 and 104.4° reported in unprotonated adenine (Voet & Rich, 1970). The imidazole and pyridine rings of the adeninium ion are coplanar.

In (I), the adeninium cations form layers parallel to the (010) plane. The Sn^{IV} atom, lying on a twofold axis, is six-coordinated and forms a quasi-regular octahedral arrangement (Bouacida *et al.*, 2005). The $[SnCl_6]^{2-}$ octahedra form anionic sheets parallel to the (010) plane, which alternate with the cationic layers along the b axis. The tilted octahedra and

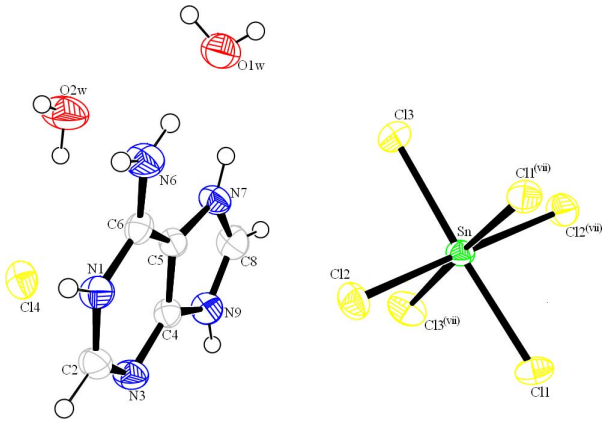


Figure 1
ORTEP-3 (Farrugia, 1997) drawing of (I) with the atomic labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (vii) $\frac{3}{2}-x, \frac{1}{2}-y, z$.]

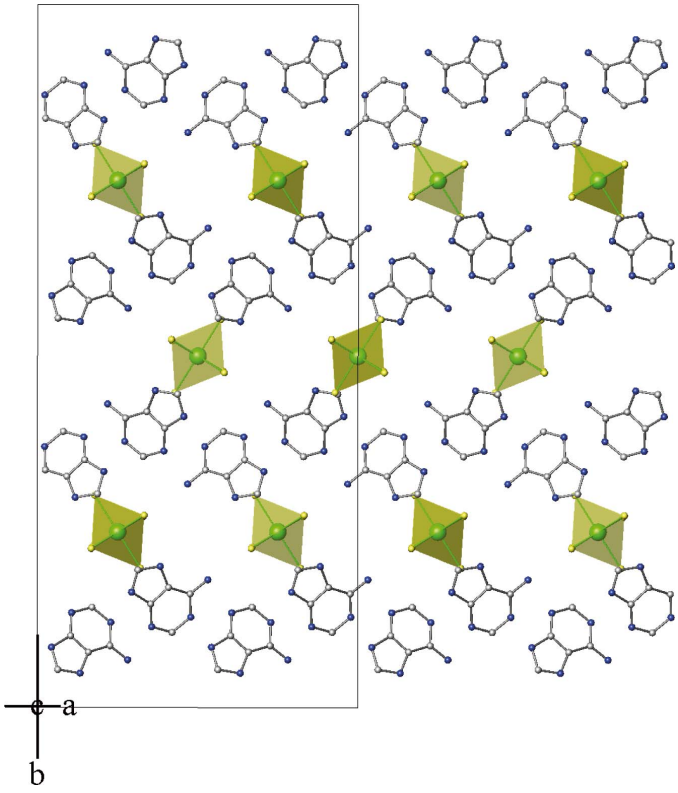


Figure 2
Packing diagram of (I), viewed down the *c* axis. H atoms, Cl^- ions and water molecules have been omitted.

layered packing are illustrated in Fig. 2. The crystal packing is mostly governed by classical hydrogen bonds (Fig. 3). Atoms N1, N6, N7, N9 and C8 of the adeninium ion participate in the formation of intermolecular and intramolecular (N—H···Cl, N—H···O and C—H···Cl) hydrogen bonds (Table 2). In this structure, we observe three types of hydrogen bonds, *viz.* cation–anion, cation–water and water–water, which form a three-dimensional network.

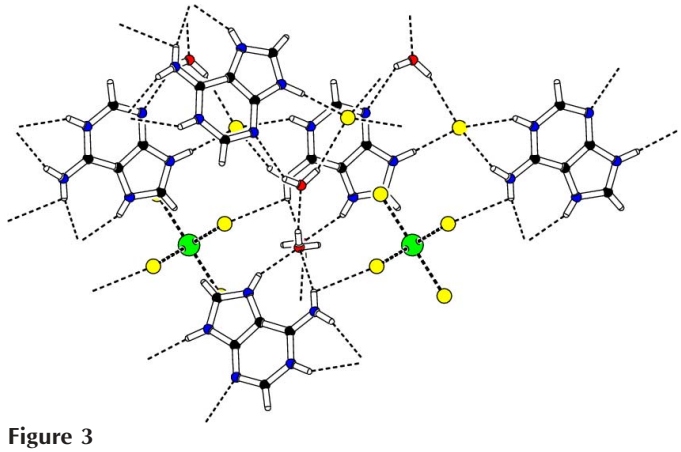


Figure 3
Part of the three-dimensional network of hydrogen bonds, shown as thin dashed lines.

Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of adenine, tin(II) oxalate and hydrochloric acid in a 10:5:1 molar ratio. Colourless prismatic crystals were obtained after one month and were manually separated for single-crystal X-ray analysis.

Crystal data

$(C_5H_7N_5)_2[SnCl_6]Cl_2\cdot 4H_2O$
$M_r = 748.67$
Orthorhombic, *Fdd*2
$a = 18.033\ (5)$ Å
$b = 39.553\ (5)$ Å
$c = 7.265\ (5)$ Å
$V = 5182\ (4)$ Å^3
$Z = 8$
$D_x = 1.919$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3316 reflections
$\theta = 2.1$–$30.0°$
$\mu = 1.85$ mm^{-1}
$T = 295$ K
Prism, colourless
0.07 × 0.06 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: none
10 885 measured reflections
3316 independent reflections
3155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 30.0°$
$h = -25 \rightarrow 25$
$k = -55 \rightarrow 37$
$l = -10 \rightarrow 6$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.061$
$S = 1.09$
3316 reflections
191 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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -1.06$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00075 (5)
Absolute structure: Flack (1983), with 1278 Friedel pairs
Flack parameter = −0.026 (17)

Table 1
Selected geometric parameters (Å, °).

Sn—Cl1	2.4419 (12)	Sn—Cl3	2.4172 (12)
Sn—Cl2	2.4252 (18)		
Cl1—Sn—Cl2	90.13 (3)	C6—N1—C2	123.8 (2)
Cl1—Sn—Cl3	176.64 (4)	C8—N7—C5	107.4 (2)
Cl2—Sn—Cl3	90.73 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl4^{i}	0.86	2.50	3.273 (2)	150
O1W—H1W···O2W^{ii}	0.71 (6)	2.08 (6)	2.782 (5)	172 (6)
O2W—H3W···Cl4	0.88 (4)	2.49 (4)	3.337 (4)	162 (3)
O2W—H4W···N3^{iii}	0.74 (6)	2.53 (6)	3.189 (5)	148 (3)
N6—H5···Cl1^{iv}	0.82 (3)	2.76 (3)	3.100 (3)	107 (2)
N6—H5···O1W	0.82 (3)	2.21 (3)	2.993 (5)	159 (3)
N6—H6···Cl4^{i}	0.92 (4)	2.33 (4)	3.205 (4)	160 (3)
N7—H7···O1W	0.82 (3)	2.01 (3)	2.766 (4)	154 (3)
N9—H9···Cl4^{v}	0.92 (4)	2.17 (4)	3.089 (3)	176 (5)
C8—H8···Cl1^{vi}	0.89 (3)	2.63 (3)	3.410 (4)	148 (3)

Symmetry codes: (i) $x-\frac{1}{4},\frac{1}{4}-y,\frac{3}{4}+z$; (ii) $1-x,\frac{1}{2}-y,\frac{1}{2}+z$; (iii) $x-\frac{1}{4},\frac{1}{4}-y,z-\frac{1}{4}$; (iv) $x-\frac{1}{2},y,z-\frac{1}{2}$; (v) $\frac{1}{4}+x,\frac{1}{4}-y,\frac{1}{4}+z$; (vi) $x,y,z-1$.

All H atoms except H1 were located in a difference Fourier map and refined isotropically. Atom H1 was placed at a calculated position, and refined using a riding model with N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *KappaCCD Reference Manual* (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), *PLUTON* (Spek, 2003) and *ATOMS* (Dowty, 1995); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Bendjeddou, L., Cherouana, A., Dahaoui, S., Benali-Cherif, N. & Lecomte, C. (2003). *Acta Cryst.* E**59**, o649–o651.
Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005). *Acta Cryst.* E**61**, m577–m579.
Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.
Cheng, Y. J.,Wang, Z. M., Liao, C. S. & Yan, C. (2002). *New J. Chem.* **26**, 1360–1364.
Dowty, E. (1995). *ATOMS.* Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hill, C. L. (1998). *Chem. Rev.* **98**, 1–2.
Hingerty, B. E., Einstein, J. R. & Wei, C. H. (1981). *Acta Cryst.* B**37**, 140–147.
Kagan, C. R., Mitzi, D. B. & Dimitrakopoulos, C. D. (1999). *Science*, **286**, 945–947.
Kistenmacher, T. J. & Shigematsu, T. (1974). *Acta Cryst.* B**30**, 166–168.
Langer, V. & Huml, K. (1978*a*). *Acta Cryst.* B**34**, 1881–1884.
Langer, V. & Huml, K. (1978*b*). *Acta Cryst.* B**34**, 1157–1163.
Langer, V., Huml, K. & Zachova, J. (1979). *Acta Cryst.* B**35**, 1148–1152.
Nonius (1998). *KappaCCD Reference Manual.* Nonius BV, Delft The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Raptopoulou, C. P., Terzis, A., Mousdis, G. A. & Papavassiliou, G. C. (2002). *Z. Naturforsch. Teil B*, **57**, 645–650.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Voet, D. & Rich, A. (1970). *Prog. Nucleic Acid Res. Mol. Biol.* **10**, 183–265.
Zeleňák, V., Vargov, Z. & Císarová, I. (2004). *Acta Cryst.* E**60**, o742–o744.