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Key indicators

Single-crystal X-ray study  
T = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
R factor = 0.041  
wR factor = 0.098  
Data-to-parameter ratio = 23.9

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

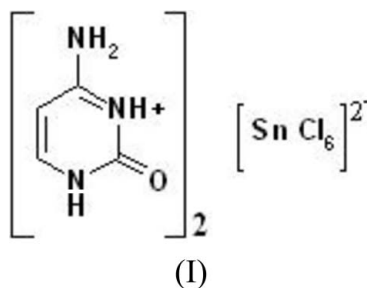
Bis(cytosinium) hexachlorostannate(IV)

The asymmetric unit of the title compound,  $(\text{C}_4\text{H}_6\text{N}_3\text{O})_2[\text{SnCl}_6]$ , contains one cytosinium cation and half a  $[\text{SnCl}_6]^{2-}$  anion, the anion lying on an inversion centre. The structure can be described as alternating layers of cytosinium and hexachlorostannate ions along the *c* axis. The packing is stabilized by N—H...Cl and N—H...O hydrogen bonding, resulting in the formation of a two-dimensional network.

Comment

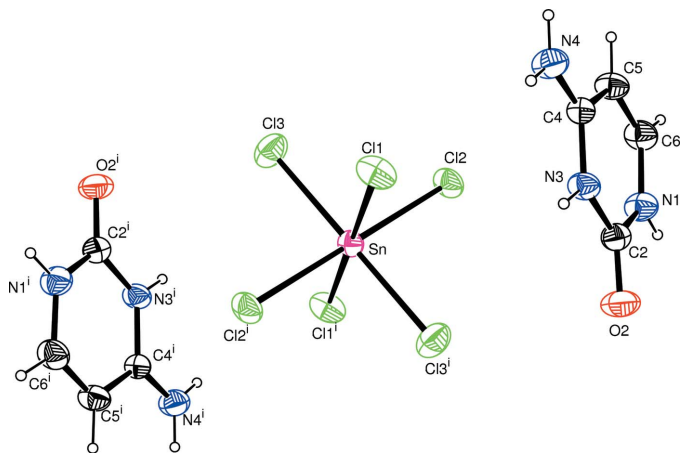
Studies of metal ion–nucleic acid interactions are of great current interest, since metal ions play a crucial role in the structure and function of nucleic acid and genetic information transfer (Salam & Aoki, 2000). The antitumour activity of organotin(IV) complexes is also known (Kabanos *et al.*, 1992).

Cytosine (6-aminopyrimidin-2-one) is one of the pyrimidines found in deoxyribonucleic acids. It has been the subject of several investigations with the aim of studying the electrostatic properties of its monohydrate form (Weber & Craven, 1990), the relative stabilities of its tautomeric forms (Kobayashi, 1998) and its hydration effects and hydrogen bonding (Sivanesan *et al.*, 2000). It offers many metal binding modes, namely *via* atom N3 (Tran Qui & Bagieu, 1990), through atom N4 (Muller *et al.*, 1998), bridging through atoms N3 and N4 (Wienkotter *et al.*, 1995), *via* atom O2 only (Cervantes *et al.*, 1990), with chelation by atoms N3 and O2 (Aoki & Saenger, 1984), and bridging through atoms N3 and O2 (Lippert *et al.*, 1984) *via* stronger N3 with additional weaker O2 interactions (Palaniandavar *et al.*, 1996). Only one crystal structure based on Sn and cytosine has been reported to date (Casellato, 1995). Here, we present a new organic–inorganic hybrid compound, (I), based on Sn and cytosine, and examine the hydrogen bonding in the crystal structure.



The title structure, (I), consists of hexachlorostannate(IV) anions lying on inversion centres and protonated cytosine rings (Fig. 1). The anionic sheet is parallel to the (001) plane and the distance between two sheets is the *c*-axis repeat. The cytosine is monoprotonated at atom N3, as previously

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**Figure 1**

A view of the title compound, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .]

reported for the tetrachlorodimethylstannate and nitrate compounds (Casellato, 1995; Cherouana *et al.*, 2003). The internal angle at N3 [ $C2-N3-C4 = 124.85 (10)^\circ$ ] is larger than the value of  $119.4^\circ$  reported in unprotonated cytosine (McClure & Craven, 1973). A similar effect has been observed in the structure of cytosinium dihydrogenmonophosphate (Bagieu-Beucher, 1990). The cations form layers parallel to the (011) plane and  $[SnCl_6]^{2-}$  octahedra alternate with the cationic layers along the  $c$  axis (Fig. 2).

The Sn atom is six-coordinated and forms a quasi-regular octahedral arrangement (Bouacida *et al.*, 2005a). This  $[SnCl_6]^{2-}$  octahedron alternates with the cationic layers along the  $c$  axis (Fig. 2). The bond lengths are similar to those found in other octahedral  $Sn^{IV}$  compounds (Bouacida *et al.*, 2005b).

The crystal packing in (I) is governed by classical hydrogen bond, in addition to coulombic forces (Fig. 3). Atoms N1, N3, N4 and C5 of the cytosine participate in the formation of strong inter- and intramolecular ( $N-H \cdots Cl$  and  $N-H \cdots O$ ) hydrogen bonds with hexachlorostannate and cytosine (Table 1), resulting in the formation of a two-dimensional network.

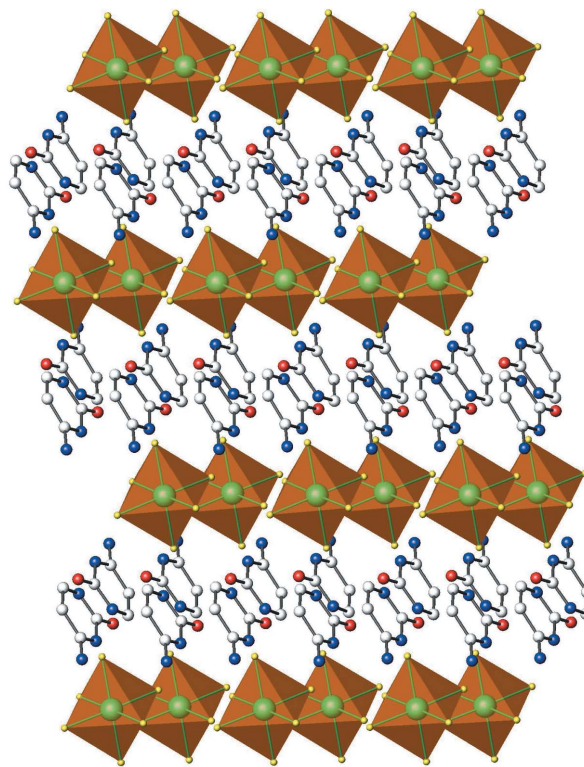
## Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of cytosine, tin(II) chloride and hydrochloric acid in a molar ratio of 10:5:1. White prismatic crystals of (I) were obtained after two weeks and were manually separated for single-crystal X-ray analysis.

### Crystal data

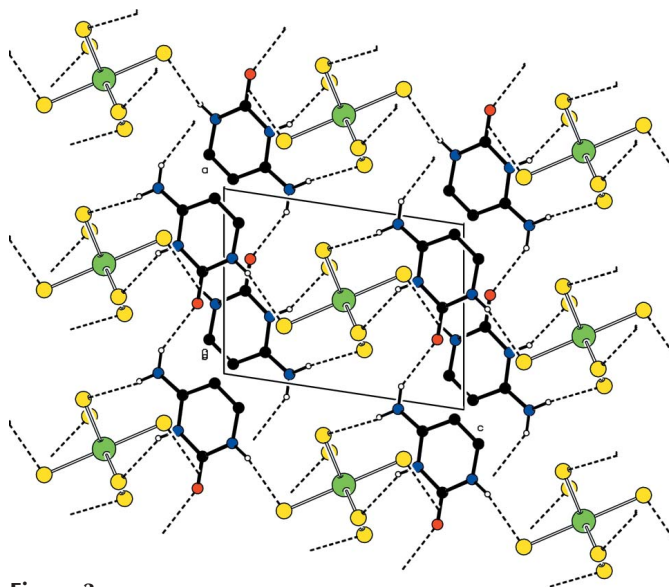
$(C_4H_6N_3O)_2[SnCl_6]$   
 $M_r = 555.63$   
 Triclinic,  $P\bar{1}$   
 $a = 6.910 (5) \text{ \AA}$   
 $b = 7.090 (5) \text{ \AA}$   
 $c = 9.270 (5) \text{ \AA}$   
 $\alpha = 101.86 (5)^\circ$   
 $\beta = 98.36 (5)^\circ$   
 $\gamma = 90.51 (5)^\circ$   
 $V = 439.4 (5) \text{ \AA}^3$

$Z = 1$   
 $D_x = 2.100 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 2533 reflections  
 $\theta = 2.3\text{--}30.1^\circ$   
 $\mu = 2.38 \text{ mm}^{-1}$   
 $T = 295 \text{ K}$   
 Prism, white  
 $0.1 \times 0.1 \times 0.1 \text{ mm}$



**Figure 2**

A diagram of the layered packing and octahedra in the title compound, viewed down the  $a$  axis.



**Figure 3**

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

### Data collection

Nonius KappaCCD area-detector diffractometer  
 $\varphi$  scans, and  $\omega$  scans with  $\kappa$  offsets  
 Absorption correction: multi-scan (SORTAV; Blessing 1995)  
 $T_{\min} = 0.717, T_{\max} = 0.792$   
 2533 measured reflections

2531 independent reflections  
 2279 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.052$   
 $\theta_{\text{max}} = 30.1^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -9 \rightarrow 9$   
 $l = -13 \rightarrow 4$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.098$   
 $S = 1.08$   
 2531 reflections  
 106 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 3.07 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.96 \text{ e } \text{\AA}^{-3}$

**Table 1**  
 Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3-H3 \cdots Cl1^i$	0.86	2.46	3.265 (4)	157
$N1-H1 \cdots Cl2^{ii}$	0.86	2.42	3.249 (4)	162
$N4-H4A \cdots Cl3^{iii}$	0.86	2.66	3.507 (4)	169
$N4-H4B \cdots O2^{iv}$	0.86	2.26	3.032 (5)	150
$N4-H4B \cdots Cl1^v$	0.86	2.92	3.490 (4)	126

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

All H atoms were located in difference Fourier maps but were introduced in calculated positions and treated as riding on their parent atoms, with  $C-H = 0.93 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ , and with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,N)$ . The very large residual electronic density has no chemical significance.

Data collection: *KappaCCD Server Software* (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), *PLATON* (Spek, 2003) and *ATOMS for Windows* (Dowty, 1995); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Aoki, K. & Saenger, W. (1984). *J. Inorg. Biochem.* **20**, 225–245.  
 Bagieu-Beucher, M. (1990). *Acta Cryst.* **C46**, 238–240.  
 Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.  
 Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005a). *Acta Cryst.* **E61**, m577–m579.  
 Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005b). *Acta Cryst.* **E61**, m1153–m1155.  
 Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.  
 Casellato, U. (1995). *Acta Cryst.* **C51**, 2293–2295.  
 Cervantes, G., Fiol, J. J., Terron, A., Moreno, V., Alabart, J. R., Aguilo, M., Gomez, M. & Solans, X. (1990). *Inorg. Chem.* **29**, 5168–5173.  
 Cherouana, A., Bouchouit, K., Bendjedou, L. & Benali-Cherif, N. (2003). *Acta Cryst.* **E59**, o983–o985.  
 Dowty, E. (1995). *ATOMS for Windows*. Version 6.0. 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.  
 Kabanos, T. A., Keramidias, A. D., Mentzafos, D., Russo, U., Terzis, A. & Tsangaris, J. M. (1992). *J. Chem. Soc. Dalton Trans.* pp. 2729–2733.  
 Kobayashi, R. (1998). *J. Phys. Chem. A*, **102**, 10813–10817.  
 Lippert, B., Thewalt, U., Schollhorn, H., Goodgame, D. M. L. & Rollins, R. W. (1984). *Inorg. Chem.* **23**, 2807–2813.  
 McClure, R. J. & Craven, B. M. (1973). *Acta Cryst.* **B29**, 1234–1238.  
 Muller, J., Zangrando, E., Pahlke, N., Freisinger, E., Randaccio, L. & Lippert, B. (1998). *Chem. Eur. J.* **4**, 397–405.  
 Nonius (1998). *KappaCCD Server Software*. 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.  
 Palaniandavar, M., Somasundaram, I., Lakshminarayanan, M. & Manohar, H. (1996). *J. Chem. Soc. Dalton Trans.* pp. 1333–1340.  
 Salam, M. A. & Aoki, K. (2000). *Inorg. Chim. Acta*, **311**, 15–24.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Sivanesan, D., Babu, K., Gadre, S. R., Subramanian, V. & Ramasami, T. (2000). *J. Phys. Chem. A*, **104**, 10887–10894.  
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
 Tran Qui, D. & Bagieu, M. (1990). *Acta Cryst.* **C46**, 1645–1647.  
 Weber, H.-P. & Craven, B. M. (1990). *Acta Cryst.* **B46**, 532–538.  
 Wienkotter, T., Sabat, M., Fusch, G. & Lippert, B. (1995). *Inorg. Chem.* **34**, 1022–1029.