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Bis(imidazolium) hexachlorostannate(IV)

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.003 Å
R factor = 0.018
wR factor = 0.046
Data-to-parameter ratio = 23.0

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

The title compound, $(C_3H_5N_2)_2[SnCl_6]$, contains discrete $[SnCl_6]^{2-}$ anions and two imidazolium $(C_3H_5N_2{}^+)$ cations. The Sn^{IV} atom is located on a center of inversion and is octahedrally coordinated by six Cl^- ions. N—H···Cl hydrogen bonds form a three-dimensional hydrogen-bonded structure.

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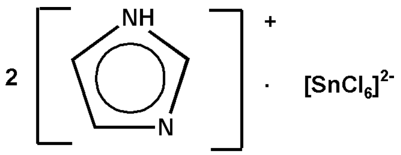
Comment

González *et al.* (1994) reported the tin and imidazolium (imH) complex $(imH)_2[Sn_2(NO_3)_4(\mu\text{-}OH)_2Me_4]$. This complex consists of imidazolium cations and $[Sn_2(NO_3)_4(\mu\text{-}OH)_2Me_4]^{2-}$ anions, with the imidazolium rings hydrogen bonded to the nitrate groups of neighbouring units and to the hydroxyl bridging groups of the anion.

The tin and imidazole (im) complexes, $Sn(im)_2Cl_2$ (Vasnin & Geanangel, 1989) and $Sn(im)_2Cl_4$ (Garnovskii *et al.*, 1966), have also been investigated.



(I)

The present structure, (I), is built up from an octahedral $[SnCl_6]^{2-}$anion and imidazolium cations. The ions are held together *via* N—H···Cl hydrogen-bonding interactions. The Sn—Cl distances range from 2.4128 (7) to 2.4470 (7) Å and the N—H···Cl from 3.318 (2) to 3.3935 (2) Å.

Experimental

$SnCl_4$ (1 mmol) and imidazole (2 mmol) were dissolved in a solution of 2 N HCl (10 ml) and the resultant solution was slowly evaporated at room temperature. The compound was obtained as prismatic colorless crystals after several days.

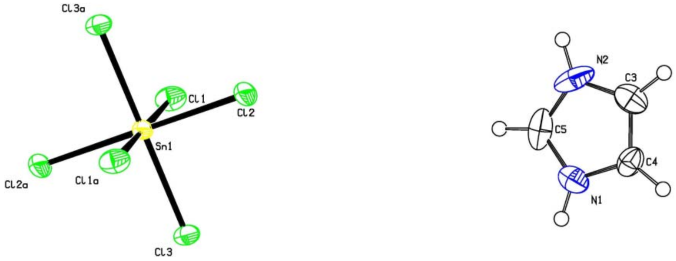


Figure 1
The unique cation and centrosymmetric anion of the title compound. Displacement ellipsoids are shown at the 50% probability level. [Symmetry code: (a) $1 - x, 2 - y, 2 - z$.]

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Crystal data

$(C_3H_5N_2)_2[SnCl_6]$
$M_r = 469.57$
Monoclinic, $P2_1/c$
$a = 7.4650$ (15) Å
$b = 8.0670$ (16) Å
$c = 12.411$ (3) Å
$\beta = 98.16$ (3)°
$V = 739.8$ (3) Å^3
$Z = 2$
$D_x = 2.108$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1820 reflections
$\theta = 2.8$–28.3°
$\mu = 2.79$ mm^{-1}
$T = 223$ (2) K
Prism, colourless
0.40 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.43$, $T_{\max} = 0.66$
9551 measured reflections
1820 independent reflections
1672 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 28.3°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.046$
$S = 1.07$
1820 reflections
79 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 0.3722P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.52$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—Cl2	2.4128 (7)	Sn1—Cl1	2.4470 (7)
Sn1—Cl3	2.4137 (8)		
Cl2—Sn1—Cl2$^{\rm i}$	180	Cl2$^{\rm i}$—Sn1—Cl1	89.507 (17)
Cl2—Sn1—Cl3	89.522 (16)	Cl3—Sn1—Cl1	90.87 (3)
Cl2$^{\rm i}$—Sn1—Cl3	90.478 (16)	Cl3$^{\rm i}$—Sn1—Cl1	89.13 (3)
Cl3—Sn1—Cl3$^{\rm i}$	180	Cl1—Sn1—Cl1$^{\rm i}$	180
Cl2—Sn1—Cl1	90.493 (17)		

Symmetry code: (i) $1 - x, 2 - y, 2 - z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl1$^{\rm ii}$	0.87	2.62	3.327 (2)	139
N1—H1···Cl2$^{\rm iii}$	0.87	2.65	3.318 (2)	135
N1—H1···Cl3$^{\rm iii}$	0.87	2.71	3.3935 (19)	137

Symmetry codes: (ii) $x, y - 1, z$; (iii) $-x, y - \frac{1}{2}, \frac{3}{2} - z$.

The H atoms were constrained to an ideal geometry, with C—H distances of 0.94 Å and N—H distances of 0.87 Å. All H atoms were refined as riding, with $U_{\rm iso}(H) = 1.2U_{\rm eq}$(parent atom).

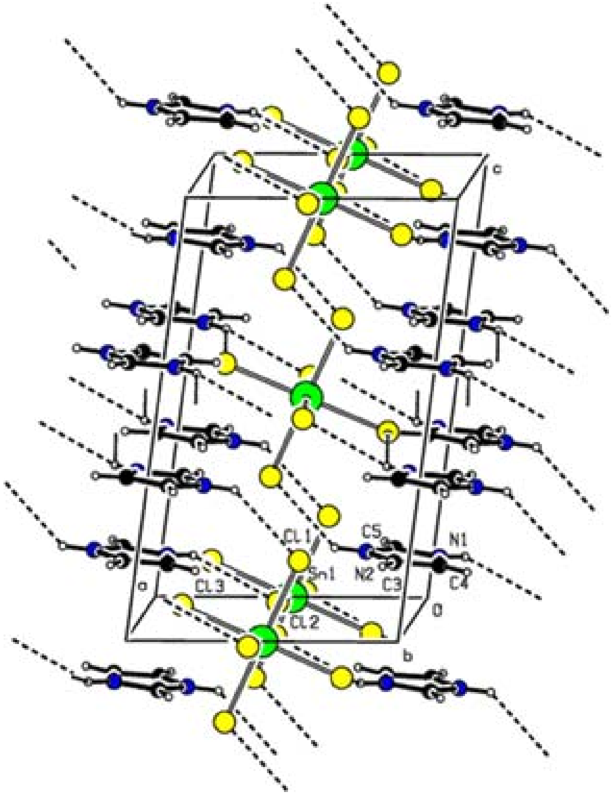

Figure 2
The crystal structure of the title compound. Dashed lines indicate hydrogen bonds

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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