

Calculations were carried out on the HITAC-M200H computer at the Computer Center of the Institute for Molecular Science with the *Universal Crystallographic Computation Program System, UNICS III* (Sakurai & Kobayashi, 1979).

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Dimethylammonium Hexachlorostannate(IV)

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Abstract. [NH₂(CH₃)₂]₂[SnCl₆], orthorhombic, *Pmnn*, *Z* = 2, *a* = 7.220 (1), *b* = 7.340 (2), *c* = 14.446 (3) Å, *V* = 765.6 (3) Å³, *D_c* = 1.837, *D_m* = 1.83 (5) Mg m⁻³; 1207 non-equivalent diffractometer data up to sin θ/λ = 0.7 Å⁻¹; final *R*(*F*) = 0.046, *R_w*(*F*) = 0.048. The structure consists of [SnCl₆]⁻ octahedra and [NH₂(CH₃)₂]⁺ groups, connected by a weak bifurcated hydrogen bond. The Sn–Cl distances corrected for libration are 2.437 (1) and 2.450 (1) Å.

Introduction. Single crystals of [NH₂(CH₃)₂]₂[SnCl₆] were obtained by slow evaporation of an acid solution containing stoichiometric amounts of [NH₂(CH₃)₂]Cl and SnCl₄. A prismatic crystal with dimensions 0.2 × 0.3 × 0.35 mm was selected for the experiments. Precession photographs showed the space group to be either *P2nn* or *Pmnn*; the latter was confirmed during the structure refinement. Data were collected in a quadrant of reciprocal space up to sin θ/λ = 0.7 Å⁻¹ with Mo *K*α radiation on a Syntex R3 diffractometer equipped with a graphite monochromator. 2661 reflections were obtained, of which 1207 were unique. Three standard reflections observed after every 100 reflections showed a gradual intensity increase of 5% during the measurement. The data were rescaled with respect to the standards. No absorption correction was performed. A weight was assigned to each reflection

according to $w(I) = [\sigma^2(I)_{\text{counting}} + (0.03I)^2]^{-1}$. The equivalent reflections were averaged [$R(I) = \sum |I - \langle I \rangle| / \sum I = 0.032$].

The structure was determined by heavy-atom and Fourier techniques. Atomic scattering factors were from *International Tables for X-ray Crystallography* (1974), except for H (Stewart, Davidson & Simpson, 1965). Anomalous-dispersion factors were applied to Sn and Cl (Cromer & Liberman, 1970). A difference synthesis showed the positions of the H atoms. They were included in the refinement, but their isotropic thermal parameters were not varied. A correction was made for secondary extinction (Larson, 1969). The structure was refined to *R*(*F*) = 0.046, *R_w*(*F*) = 0.048 and *S* = $[\sum w(F_o - F_c)^2 / (\text{NO} - \text{NV})]^{1/2} = 2.65$.*

The calculations were carried out with the XRAY system (Stewart, Kruger, Ammon, Dickinson & Hall, 1972) on the Univac 1108 computer of the University of Frankfurt. The positional parameters of the atoms are reported in Table 1, bond lengths and angles in Table 2.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36015 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Positional parameters and equivalent values of the anisotropic temperature factor ($U_{eq} = \frac{1}{3} \text{trace } U$)

	x	y	z	U_{eq} (Å ²)
Sn	0.0	0.0	0.0	0.036 (1)
Cl(1)	0.0	0.17854 (18)	0.14195 (8)	0.063 (1)
Cl(2)	0.24124 (11)	0.19241 (11)	-0.06378 (5)	0.056 (1)
N	0.0	0.6877 (6)	0.3626 (3)	0.054 (2)
C(1)	0.0	0.8863 (8)	0.3637 (6)	0.088 (5)
C(2)	0.0	0.6004 (11)	0.2728 (4)	0.076 (4)
H(1)	0.086 (6)	0.652 (4)	0.398 (3)	0.055*
H(2)	0.0	0.483 (8)	0.281 (5)	0.085*
H(3)	0.118 (7)	0.653 (5)	0.246 (4)	0.085*
H(4)	0.0	0.958 (9)	0.437 (5)	0.090*
H(5)	0.099 (8)	0.927 (7)	0.331 (3)	0.090*

* Not refined.

Table 2. Bond distances (Å) and angles (°)

2 × Sn—Cl(1)	2.434 (1)	Cl(1)—Sn—Cl(2)	90.37 (3)
	[2.450 (1)]*	Cl(1)—Sn—Cl(2)	89.63 (3)
4 × Sn—Cl(2)	2.424 (1)	Cl(2)—Sn—Cl(2)	88.14 (3)
	[2.437 (1)]	Cl(2)—Sn—Cl(2)	91.86 (3)
1 × N—C(1)	1.458 (7)	C(1)—N—C(2)	116.9 (5)
1 × N—C(2)	1.447 (7)	C(1)—N—H(1)	108 (2)
2 × N—H(1)	0.85 (4)	C(2)—N—H(1)	114 (2)
1 × C(1)—H(4)	1.18 (8)	H(1)—N—H(1)	94 (4)
2 × C(1)—H(5)	0.91 (5)		
1 × C(2)—H(2)	0.87 (6)		
2 × C(2)—H(3)	1.01 (5)		

* Values in square brackets are corrected for libration.

Discussion. A stereoscopic view of the structure is shown in Fig. 1. The structure consists of $[\text{SnCl}_6]^-$ octahedra and $[\text{NH}_2(\text{CH}_3)_2]^+$ groups. The two independent Sn—Cl bonds, corrected for libration (Schomaker & Trueblood, 1968), are, respectively, 2.437 (1) and 2.450 (1) Å. They agree well with the values of 2.426 and 2.428 Å in the corresponding K^+ and NH_4^+ compounds (Lerbscher & Trotter, 1976) and the values of 2.404 to 2.447 Å in the $[\text{N}(\text{C}_2\text{H}_5)_4]^+$ analogue (Sowa, Drück & Kutoglu, 1981). The packing of the structure consists of a bifurcated hydrogen bond between H(1) and Cl(2), reported in Table 3. The H(1)···Cl(2) distances of 2.87 (3) and 2.72 (4) Å are rather long. Therefore, the hydrogen bonds have to be classified as weak.

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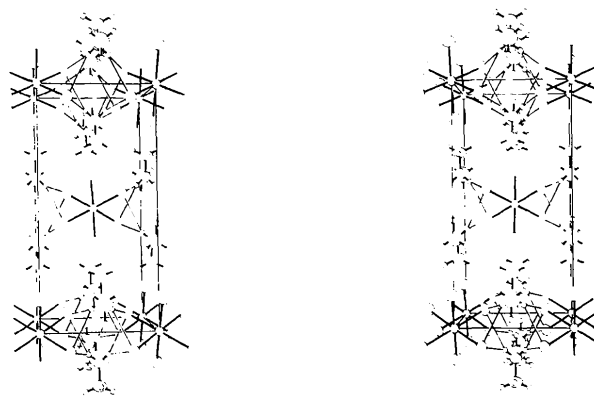
Fig. 1. Stereoscopic view of the structure along **b**. The thermal ellipsoids correspond to the 50% probability surfaces.

Table 3. Hydrogen bonds

N—H···Cl	H···Cl (Å)	N···Cl (Å)	∠N—H···Cl (°)
N—H(1)···Cl(2) ^a	2.87 (3)	3.522 (4)	135 (3)
N—H(1)···Cl(2) ^b	2.72 (4)	3.455 (3)	147 (3)

Symmetry code

(a) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z$ (b) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$

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