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(2-Dimethylaminoethyl)dimethylammonium dichlorotrimethylstannate(IV)

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Key indicators

Single-crystal X-ray study
T = 140 K
Mean σ(C–C) = 0.007 Å
R factor = 0.033
wR factor = 0.085
Data-to-parameter ratio = 22.6

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

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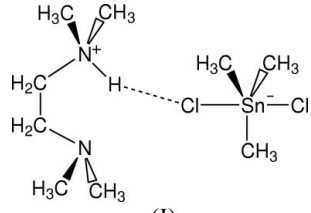
The structure of the title compound, $(C_6H_{17}N_2)[SnCl_2(CH_3)_2]$, shows an anion–cation contact *via* a hydrogen bond. The stannate anion is five-coordinate. There are two cations and two anions in the asymmetric unit.

Comment

(2-Dimethylaminoethyl)dimethylammonium dichlorotrimethylstannate(IV), (I), crystallizes in the monoclinic space group $P2_1/c$ with eight molecules per unit cell. The asymmetric unit contains two almost identical cation–anion pairs that differ only in their hydrogen bonding. Each Sn atom is five-coordinate. Only one stannate ion displays hydrogen bonding, with interatomic distances of N1—H1* = 1.02 (4) Å, H1*—Cl1 = 2.28 (4) Å, N3—H3* = 0.96 (4) Å and H3*—Cl2 = 2.55 (4) Å. The second stannate ion does not show interactions with polar H atoms. For comparison, 2,2′-iminodipyridinium dichlorotriphenylstannate(IV) exhibits an H···Cl bond length of 2.291 Å (Ng, 1999). The bond lengths and angles of (I) are in good agreement with those of bis(trimethylstannyl)ammonium dichlorotrimethylstannate(IV) (Hillwig *et al.*, 1997) and 2,2,6,6-tetramethylpiperidinium dichlorotrimethylstannate(IV) (Johnson *et al.*, 1991).



(I)

Experimental

The title compound was isolated as a byproduct after a reaction of HCl, formed in an elimination reaction, with traces of chlorotrimethyltin and TMEDA. It was isolated as colourless needles by crystallization from toluene at 253 K.

Crystal data

$(C_6H_{17}N_2)[SnCl_2(CH_3)_2]$
M_r = 351.91
Monoclinic, $P2_1/c$
a = 14.480 (3) Å
b = 12.278 (3) Å
c = 19.366 (4) Å
β = 107.41 (3)°
V = 3285.3 (11) Å^3
Z = 8
D_x = 1.423 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 225 reflections
θ = 2.7–22.7°
μ = 1.86 mm^{-1}
T = 140 (1) K
Needle, colourless
0.3 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS-IIc diffractometer
φ scans (46 frames with 4° oscillation were recorded)
11 409 measured reflections
6025 independent reflections
4747 reflections with $I > 2\sigma(I)$

$R_{int} = 0.027$
$\theta_{max} = 25.4°$
$h = -17 \rightarrow 17$
$k = -14 \rightarrow 14$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.085$
$S = 1.03$
6025 reflections
267 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.92$ e Å^{-3}

H atoms bounded to N atoms were located in a difference map and allowed to refine freely. The other H atoms in the cation were included in idealized positions and their U_{iso} values were set to ride on the U_{eq} values of the parent C atom. H atoms in the anion were placed in idealized positions, set to ride on the parent C atoms and allowed to rotate about the Sn—C bond.

Data collection: *MSC R-AXIS*-II *Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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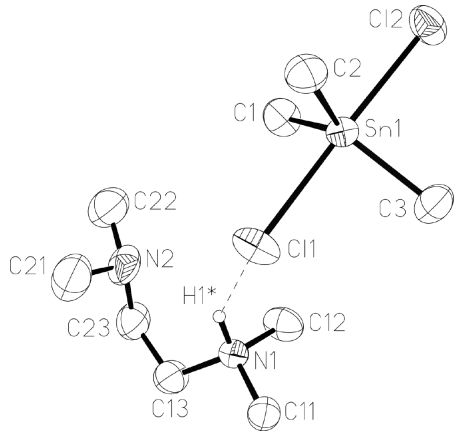

Figure 1
A view of (I). Displacement ellipsoids are drawn here at the 50% probability level.

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