Crystal structure of the bis(2-amino-1,3-dimethylimidazolium)chloride trichlorostannate, $[\text{C}_5\text{H}_{10}\text{N}_3]^+\text{SnCl}_3^- \cdot [\text{C}_5\text{H}_{10}\text{N}_3]^+\text{Cl}^-$

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.40 x 0.40 x 0.45 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	19.45 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	173 K
$2\theta_{\text{max}}$:	90.9°
$N(hkl)_{\text{unique}}$:	3298
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	191
Program:	SHELXTL-plus

Source of material: See ref. 1.

Selected bond lengths and angles: Sn(1)–Cl(1) 2.501(1) Å, Sn(1)–Cl(2) 2.510(1) Å, Sn(1)–Cl(3) 2.512(1) Å, Cl(1)–Sn(1)–Cl(2) 92.86(5)°, Cl(1)–Sn(1)–Cl(3) 91.58(4)°, Cl(2)–Sn(1)–Cl(3) 92.55(4)°.

$\text{C}_{10}\text{H}_{20}\text{Cl}_4\text{N}_6\text{Sn}$, monoclinic, $P2_1/n1$ (No. 14), $a = 14.043(3)$ Å, $b = 8.674(6)$ Å, $c = 16.815(3)$ Å, $\beta = 114.45(1)^\circ$, $V = 1864.6$ Å³, $Z = 4$, $R(F) = 0.053$, $R_w(F) = 0.127$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(4A)	4e	0.7184(3)	0.9188(4)	0.3251(2)	0.039
H(4B)	4e	0.6719(3)	0.7584(4)	0.2979(2)	0.039
H(3A)	4e	0.3029(3)	0.0716(5)	0.0054(3)	0.043
H(8A)	4e	0.5406(3)	0.7182(5)	0.5122(3)	0.039
H(7A)	4e	0.6152(3)	0.9767(5)	0.5544(2)	0.036
H(1A)	4e	0.5039(4)	−0.3677(5)	−0.0513(2)	0.053
H(1B)	4e	0.4949(4)	−0.3814(5)	0.0357(2)	0.053
H(9A)	4e	0.7077(4)	1.1724(5)	0.4964(3)	0.048
H(9B)	4e	0.6587(4)	1.1582(5)	0.3922(3)	0.048
H(9C)	4e	0.7754(4)	1.0996(5)	0.4491(3)	0.048
H(2A)	4e	0.3169(3)	0.0956(5)	−0.1353(3)	0.041
H(5A)	4e	0.3558(4)	−0.1317(6)	0.1287(3)	0.048
H(5B)	4e	0.4629(4)	−0.2179(6)	0.1445(3)	0.048
H(5C)	4e	0.3533(4)	−0.3007(6)	0.0897(3)	0.048
H(10A)	4e	0.5259(3)	0.5197(5)	0.3935(3)	0.043
H(10B)	4e	0.6222(3)	0.5253(5)	0.3662(3)	0.043
H(10C)	4e	0.5138(3)	0.6062(5)	0.3058(3)	0.043
H(4C)	4e	0.4046(4)	−0.0643(5)	−0.2173(3)	0.046
H(4D)	4e	0.4032(4)	−0.2450(5)	−0.1985(3)	0.046
H(4E)	4e	0.5086(4)	−0.1479(5)	−0.1506(3)	0.046

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Sn(1)	4e	0.26780(2)	0.22049(3)	0.24539(2)	0.0338(3)	0.0282(3)	0.0227(2)	0.00316(8)	0.0128(2)	−0.00063(8)
Cl(1)	4e	0.35293(9)	0.4061(1)	0.18124(7)	0.0468(6)	0.0370(5)	0.0418(5)	−0.0107(4)	0.0135(4)	0.0057(4)
Cl(2)	4e	0.42170(8)	0.0409(1)	0.29656(6)	0.0372(5)	0.0533(6)	0.0244(4)	0.0133(4)	0.0129(4)	0.0087(4)
Cl(3)	4e	0.17968(7)	0.0820(1)	0.10207(6)	0.0323(5)	0.0397(5)	0.0267(5)	−0.0031(3)	0.0107(4)	−0.0054(3)
Cl(4)	4e	0.64553(8)	−0.4212(1)	0.18367(5)	0.0391(5)	0.0343(5)	0.0216(4)	0.0052(3)	0.0134(4)	−0.0029(3)
N(6)	4e	0.5982(3)	0.7269(4)	0.4154(2)	0.026(2)	0.033(2)	0.020(2)	−0.001(1)	0.011(1)	0.001(1)
N(3)	4e	0.3878(3)	−0.1339(4)	0.0222(2)	0.033(2)	0.028(2)	0.023(1)	−0.001(1)	0.011(1)	0.002(1)
C(1)	4e	0.4279(3)	−0.1992(4)	−0.0295(2)	0.033(2)	0.027(2)	0.019(2)	−0.003(1)	0.007(2)	−0.001(1)
N(2)	4e	0.4025(3)	−0.1114(4)	−0.1008(2)	0.030(2)	0.028(2)	0.024(1)	−0.001(1)	0.009(1)	0.004(1)
C(6)	4e	0.6507(3)	0.8403(4)	0.3965(2)	0.024(2)	0.030(2)	0.018(1)	−0.001(1)	0.007(1)	0.002(1)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(5)	4e	0.6649(2)	0.9565(4)	0.4530(2)	0.031(2)	0.030(2)	0.018(1)	0.000(1)	0.011(1)	−0.002(1)
N(4)	4e	0.6842(3)	0.8390(4)	0.3325(2)	0.045(2)	0.031(2)	0.031(2)	−0.009(1)	0.027(1)	−0.010(1)
C(3)	4e	0.3371(3)	0.0015(5)	−0.0175(3)	0.032(2)	0.037(2)	0.039(2)	0.009(2)	0.015(2)	0.006(2)
C(8)	4e	0.5773(3)	0.7752(5)	0.4855(3)	0.033(2)	0.046(2)	0.022(2)	0.001(2)	0.016(2)	0.003(2)
C(7)	4e	0.6178(3)	0.9156(5)	0.5085(2)	0.032(2)	0.041(2)	0.018(2)	0.003(2)	0.012(1)	0.000(1)
N(1)	4e	0.4817(4)	−0.3311(5)	−0.0132(2)	0.073(3)	0.030(2)	0.025(2)	0.016(2)	0.016(2)	0.001(1)
C(9)	4e	0.7050(4)	1.1092(5)	0.4472(3)	0.063(3)	0.029(2)	0.036(2)	−0.012(2)	0.030(2)	−0.012(2)
C(2)	4e	0.3450(3)	0.0151(5)	−0.0938(3)	0.035(2)	0.033(2)	0.035(2)	0.008(2)	0.015(2)	0.009(2)
C(5)	4e	0.3901(4)	−0.2017(6)	0.1030(3)	0.054(3)	0.044(2)	0.026(2)	0.002(2)	0.020(2)	0.007(2)
C(10)	4e	0.5620(3)	0.5824(5)	0.3661(3)	0.036(2)	0.039(2)	0.039(2)	−0.010(2)	0.021(2)	−0.009(2)
C(4)	4e	0.4321(4)	−0.1449(5)	−0.1727(3)	0.047(2)	0.042(2)	0.027(2)	0.005(2)	0.017(2)	0.004(2)

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References

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