Crystal structure of chlorodimethyl(2-aminoethanethiolato)tin(IV), $(\text{NH}_2\text{CH}_2\text{CH}_2\text{S})\text{SnCl}(\text{CH}_3)_2$

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Abstract

$\text{C}_4\text{H}_{12}\text{ClNSSn}$, orthorhombic, $Pbca$ (no. 61), $a = 11.422(2)$ Å, $b = 11.475(2)$ Å, $c = 13.582(2)$ Å, $V = 1780.2$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.057$, $wR_{\text{ref}}(F^2) = 0.147$, $T = 293$ K.

Source of material

The title compound was synthesized by adding a suspension of dimethyl tin(IV) oxide (4 mmol) in EtOH to a solution 2-aminoethanethiol hydrochloride in EtOH in 1:1 molar ratio and stirring the mixture for 6 h at 60 °C. On cooling, colorless crystals of the compound were formed suitable for the structural study (yield 65 %, m.p. 200 °C). Elemental analysis: found – C, 18.8 %; H, 4.9 %; N, 5.3 %; S, 12.0 %; calc. for $\text{C}_4\text{H}_{12}\text{ClNSSn}$ – C, 18.5 %; H, 4.7 %; N, 5.4 %; S, 12.3 %. In a similar way the bromine analogue was prepared (yield 70 %, m.p. 196 °C).

Discussion

The biological activity of complexes of tin and organotin moieties with ligands containing S and N donor atoms can be influenced by the nature of the ligand. Owing to the importance of aminoethanethiols in biological systems we prepared some organotin complexes with both 2-aminoethanethiol (cysteamine) and 2-dimethylaminoethanethiol. We report here on the structure of chlorodimethyl(2-aminoethanethiolato)tin(IV).

Two carbon and one sulphur atom form the trigonal base of the coordination bipyramid around the tin metal atom. Distortions from the trigonal bipyramidal idealized geometry are essentially due to bond angles involving the nitrogen atom: $\angle \text{Cl}–\text{Sn}–\text{N} =$

$167.3(1)^\circ$ and $\angle \text{S}–\text{Sn}–\text{N} = 80.8(1)^\circ$, probably because its position is constrained by the structure of the chelate ligand. The equatorial coordination distances, $d(\text{Sn}–\text{S}) = 2.415(2)$ Å, $d(\text{Sn}–\text{C}) = 2.118(6)$ Å and $2.119(6)$ Å, agree well with the sum of the corresponding covalent or atomic radii, while the apical distances $d(\text{Sn}–\text{Cl}) = 2.593(2)$ Å and $d(\text{Sn}–\text{N}) = 2.309(5)$ Å are considerably longer. All other structural data are as expected and resemble those reported for chlorodiethyl(2-dimethylaminoethanethiolato)tin(IV) [1]. Small differences are observed in the Sn–Cl and Sn–N bond distances, that are $2.544(2)$ Å and $2.388(7)$ Å in the cited compound, whereas the Sn–S distances have the same value. A very long Sn–N distance of $2.647(2)$ Å was found in bis(triphenyl)chlorodimethyl(2-aminoethanethiolato)tin(IV) [2], where the tin atom is four-coordinated, and a value of $2.43(1)$ Å was reported for the ethyl L-cysteinato derivative [3].

Table 1. Data collection and handling.

Crystal:	colorless prism, size $0.12 \times 0.20 \times 0.25$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71070 Å)
μ :	33.22 cm^{-1}
Diffractometer, scan mode:	Philips PW 1100, θ – 2θ
$2\theta_{\text{max}}$:	56°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2146, 2146
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1633
$N(\text{param})_{\text{refined}}$:	73
Programs:	SHELXS-97 [4], SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1N)	8c	0.1586	–0.0243	0.1843	0.044
H(2N)	8c	0.0392	–0.0072	0.1487	0.044
H(1A)	8c	0.1219	0.2024	0.4102	0.082
H(1B)	8c	0.1818	0.0887	0.3708	0.082
H(1C)	8c	0.0450	0.0961	0.3775	0.082
H(2A)	8c	–0.1016	0.1916	0.1468	0.079
H(2B)	8c	–0.0284	0.2721	0.0766	0.079
H(2C)	8c	–0.0797	0.3223	0.1749	0.079
H(3A)	8c	0.1027	0.0808	0.0093	0.051
H(3B)	8c	0.1607	–0.0430	0.0181	0.051
H(4A)	8c	0.3000	0.1018	–0.0178	0.049
H(4B)	8c	0.3296	0.0353	0.0798	0.049

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Table 3. 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)	8c	0.10884(3)	0.20642(3)	0.21909(3)	0.0258(3)	0.0325(3)	0.0327(3)	0.0018(1)	0.0004(1)	0.0015(1)
S(1)	8c	0.2796(1)	0.2270(1)	0.1156(1)	0.0374(8)	0.0367(7)	0.0543(9)	−0.0092(6)	0.0131(7)	−0.0067(6)
Cl(1)	8c	0.1511(2)	0.4166(1)	0.2797(1)	0.0453(9)	0.0367(8)	0.058(1)	−0.0021(6)	0.0091(7)	−0.0110(6)
N(1)	8c	0.1119(4)	0.0232(4)	0.1492(4)	0.035(3)	0.030(2)	0.046(3)	−0.003(2)	0.002(2)	0.004(2)
C(1)	8c	0.1152(6)	0.1392(7)	0.3642(5)	0.062(4)	0.058(5)	0.044(3)	0.002(3)	−0.002(3)	0.009(3)
C(2)	8c	−0.0465(6)	0.2547(7)	0.1441(5)	0.035(3)	0.070(4)	0.054(4)	0.016(3)	−0.011(3)	0.002(3)
C(3)	8c	0.1559(6)	0.0336(5)	0.0481(4)	0.049(3)	0.036(3)	0.043(3)	−0.003(3)	0.000(3)	−0.005(2)
C(4)	8c	0.2747(5)	0.0889(5)	0.0495(4)	0.040(3)	0.038(3)	0.045(3)	−0.004(2)	0.015(2)	−0.007(2)

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