Crystal structure of dichlorobis(4-amino-1,2,4-triazole)dimethyltin(IV), $SnCl_2(CH_3)_2(C_2H_4N_4)_2$

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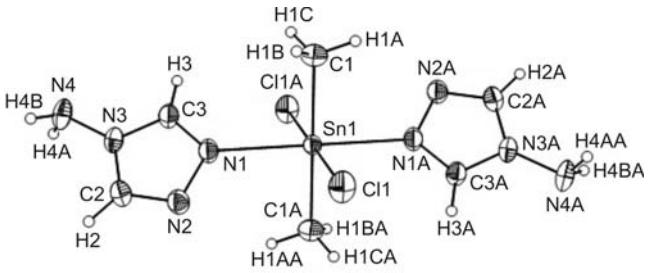

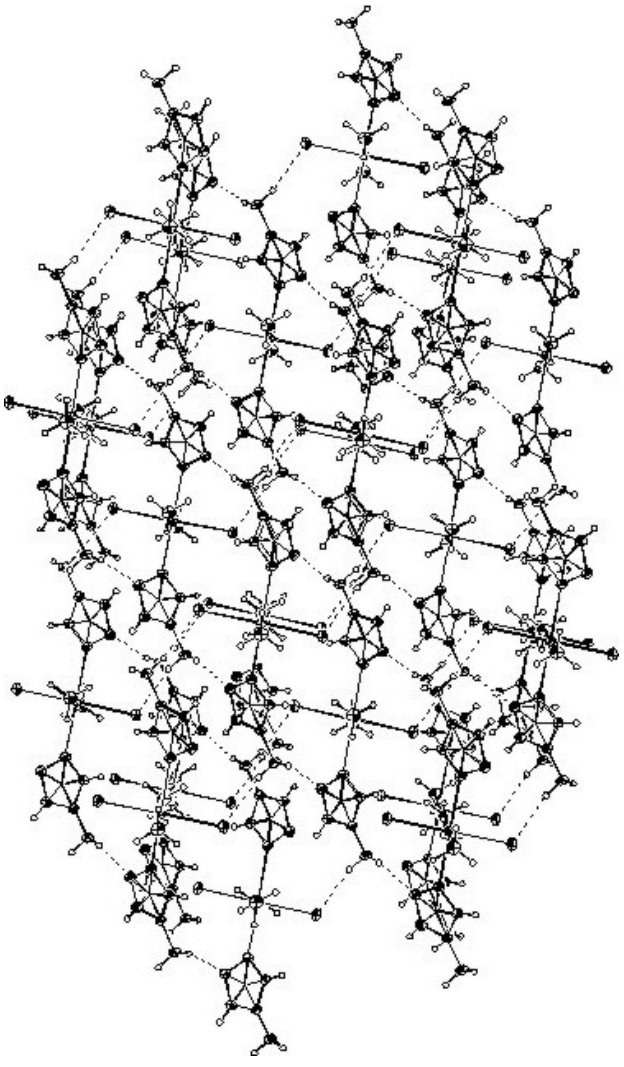

Abstract

$C_6H_{14}Cl_2N_8Sn$, monoclinic, $P12_1/c1$ (no. 14), a = 8.689(2) Å, b = 7.524(3) Å, c = 11.359(3) Å, β = 109.86(1)°, V = 698.5 Å^3, Z = 2, $R_{gf}(F)$ = 0.023, $wR_{ref}(F^2)$ = 0.057, T = 293 K.

Source of material

To a solution of 4-amino-1,2,4-triazole (0.824 g, 9.8 mmol) in 10 ml methanol, a solution of dimethyltin dichloride (1.076 g, 4.9 mmol) in 5 ml methanol was added dropwise. The clear solution was stirred under reflux condition for 24 h. Colorless crystals were obtained after one day in refrigerator.

Experimental details

Hydrogens bound to nitrogen atoms were found in difference Fourier maps and refined freely. All the other hydrogen atoms were placed geometrically.

Discussion

Organotin(IV) complexes have attracted attention because of their versatile biological properties [1,2] as well as their industrial and agricultural applications [3]. Triazole derivatives also display a broad range of biological activity, showing potential applications as antitumor, antibacterial, antifungal and antiviral agents [4].

The Sn coordination in the title complex is octahedral with 4-amino-1,2,4-triazole ligands in a *trans* fashion; the chlorine atoms are also *trans* (figure, top). The Sn atom is located in the inversion centre. 4-Amino-1,2,4-triazole ligands linked to Sn via N1 nitrogen atom of triazole ring. The Sn—N, Sn—Cl and Sn—C bond lengths are within expected values [2.358(2), 2.5808(9) and 2.107(2) Å, respectively]. The N–Sn–N angle is 180° and the Sn–N–N angle is 123.7(1)°. N1 atom is within the plane of the aminotriazole molecule but the Sn is not within in this plane. Thus the environment of N1 atom deviates from planarity: the torsion angle N3–C3–N1–Sn1 is 166.0(1)°. The N–H···N (d(N4···N2) = 3.109(3) Å) and N–H···Cl (d(N4···Cl1) = 3.303(2) Å) hydrogen bonds, Cl···π (d(Cl1···centroid) = 3.631(2) Å) and π···π contacts (d(centroid···centroid) = 3.522(2) Å) are responsible for aggregation of molecules in a 3D arrangement (figure, bottom).

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Table 1. Data collection and handling.

Crystal:	colorless block, size 0.35 × 0.46 × 0.59 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	22.05 cm^{-1}
Diffractometer, scan mode:	Kappa CCD,
$2\theta_{max}$:	56.4°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6263, 1517
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1322
$N(param)_{refined}$:	89
Programs:	SHELXS-97, SHELXL-97 [5], DIAMOND [6], WinGX [7]

Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	4*e*	1.049	0.6624	0.4851	0.065
H(1B)	4*e*	0.8641	0.6890	0.4695	0.065
H(1C)	4*e*	0.9977	0.6934	0.6032	0.065
H(2)	4*e*	0.4839	1.2676	0.5765	0.043
H(3)	4*e*	0.8223	0.9111	0.7229	0.039
H(4A)	4*e*	0.612(3)	1.150(3)	0.845(2)	0.069(9)
H(4B)	4*e*	0.471(2)	1.051(4)	0.763(3)	0.061(8)

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.9742(3)	0.7236(3)	0.5167(2)	0.051(1)	0.030(1)	0.051(1)	0.0008(9)	0.021(1)	0.0025(9)
C(2)	4*e*	0.5719(2)	1.1909(3)	0.5885(2)	0.0313(9)	0.042(1)	0.035(1)	0.0047(8)	0.0136(8)	–0.0033(8)
C(3)	4*e*	0.7571(3)	0.9961(2)	0.6695(2)	0.029(1)	0.042(1)	0.030(1)	0.0031(7)	0.0122(9)	0.0018(7)
N(1)	4*e*	0.7737(2)	1.0498(3)	0.5657(2)	0.0318(9)	0.0410(8)	0.0311(9)	0.0061(7)	0.0155(7)	0.0023(7)
N(2)	4*e*	0.6532(2)	1.1748(2)	0.5118(2)	0.0357(8)	0.0419(9)	0.0310(9)	0.0071(7)	0.0137(7)	0.0025(7)
N(3)	4*e*	0.6324(2)	1.0813(2)	0.6882(2)	0.0295(8)	0.0403(9)	0.0272(9)	–0.0039(7)	0.0135(6)	–0.0057(7)
N(4)	4*e*	0.5820(3)	1.0552(3)	0.7925(2)	0.040(1)	0.066(1)	0.032(1)	–0.005(1)	0.0224(8)	–0.005(1)
Cl(1)	4*e*	0.81592(8)	0.98494(8)	0.26783(6)	0.0342(3)	0.0646(4)	0.0286(3)	0.0033(2)	0.0049(2)	–0.0010(2)
Sn(1)	2*c*	0	0	½	0.0252(2)	0.0267(2)	0.0242(2)	0.00164(5)	0.01007(9)	–0.00004(5)

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