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Crystal structure of dichloro-bis(*n*-pentyl)tin(IV), $Sn(C_5H_{11})_2Cl_2$, *tin-halide compounds – part VI*

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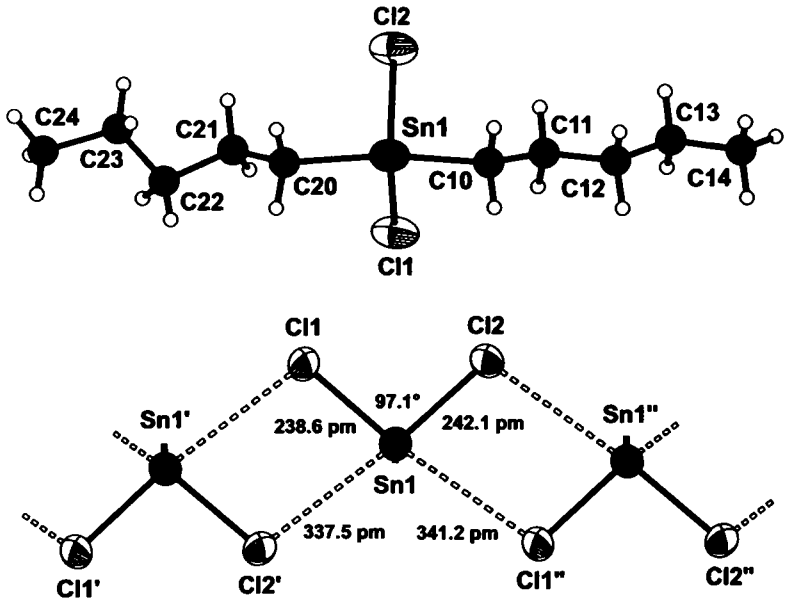

Abstract

$C_{10}H_{22}Cl_2Sn$, orthorhombic, $P2_12_12_1$ (no. 19), a = 6.5566(6) Å, b = 9.068(1) Å, c = 25.316(2) Å, V = 1505.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.062, $wR_{ref}(F^2)$ = 0.167, T = 258 K.

Source of material

The title compound was synthesized according to published procedure [1]. Suitable single crystals were grown from the melt.

Experimental details

Because of the high flexibility of the *n*-pentyl rest high anisotropic thermal parameters resulted for all carbon atoms. Because this effect distorted some of the bond lengths and angles all carbon atoms were refined isotropically in addition to a common carbon-carbon bond length. Moreover, the most prominent disordering of side chain 2 was taken into account by a second position of the methylene groups C22, C23 and the methyl group C24 with side occupancy factors for both conformations of 0.75 and 0.25, respectively.

Discussion

Diorganotin dichlorides are versatile tools for the preparation of other organotin compounds. The most interesting structural features of their solid state structures result from the intermolecular interaction of the polar molecules which show in solutions of non complexing solvents a tetrahedral coordination of the tin atom. In the title compound (figure, top) this intermolecular interaction leads to an antiparallel orientation of the dipol moments of the individual ^{n}Pe$_2$SnCl$_2$ molecules thus forming linear chains along the *b* axis (figure, bottom).

Among the dialkyltin dichlorides, R_2SnCl_2, those with unbranched chains (R = Me [2], Et [3], ^{n}Bu [4]) adopt the same arrangement as the title compound with its unbranched *n*-pentyl rest. Probably as a result of this interaction, there are significant angular distortions in the individual molecules as well as changes of the tin-chlorine bond lengths. Angular distortions from tetrahedral values are best described with respect to the C–Sn–C and Cl–Sn–Cl angles which are widened and reduced, respectively. The corresponding values are 139.6(5)°/97.1(2)° in the title compound and 142.2°/98.6° (R = Me), 133.8°/96.0° (R = Et) and 132.1°/97.2° (R = ^{n}Bu). On the other hand intramolecular tin-chlorine bond lengths depend from the extend of the intermolecular interaction which is best described by the intermolecular tin···chlorine distances. The actual values are 242.1(4) pm/238.6(4) pm (average value 240.4 pm) for the intramolecular bonds and 341.2 pm/337.5 pm (average value 339.4 pm) for the intermolecular distances. The corresponding average values of the other compounds are 238.9 pm/343.3 pm (R = Me), 238.6 pm/346.2 pm (R = Et), and 238.1 pm/352.9 pm (R = ^{n}Bu). There is a direct correlation between both bond lengths: the shorter the intermolecular contact the longer the intramolecular bonds. Dialkyltin dichlorides with branched alkyl groups adopt a somewhat different type of structure (R = ^{i}Pr [5]) or represent monomeric molecules in solid state (R = ^{t}Bu [5]). In ^{t}Bu$_2$SnCl$_2$ there is no intermolecular contact shorter than 460 pm. In this case the average intramolecular tin-chlorine bond length is 233.5 pm, and the values of the angles C–Sn–C and Cl–Sn–Cl are 101.9° and 133.1°, respectively.

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Table 1. Data collection and handling.

Crystal:	colorless transparent needle, size 0.12 × 0.13 × 0.15 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	20.18 cm^{-1}
Diffractometer, scan mode:	Siemens P4, $\omega/2\theta$
$2\theta_{max}$:	41.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1860, 1554
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1461
$N(param)_{refined}$:	73
Programs:	SHELXS-97 [6], SHELXL-97 [7], DIAMOND [8], SHELXTL [9]

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

Atom	Site	Occ.	x	y	z	U_{iso}
C(10)	4*a*		0.595(2)	0.362(2)	0.8271(6)	0.071(4)
H(101)	4*a*		0.5346	0.4485	0.8435	0.20(3)
H(102)	4*a*		0.5357	0.2755	0.8432	0.20
C(11)	4*a*		0.822(2)	0.363(2)	0.8371(5)	0.080(5)
H(111)	4*a*		0.8828	0.2792	0.8193	0.20
H(112)	4*a*		0.8801	0.4519	0.8220	0.20
C(12)	4*a*		0.874(2)	0.356(2)	0.8949(5)	0.087(5)
H(121)	4*a*		0.8351	0.2606	0.9087	0.20
H(122)	4*a*		0.7953	0.4305	0.9136	0.20
C(13)	4*a*		1.097(2)	0.381(3)	0.9053(7)	0.108(7)
H(131)	4*a*		1.1769	0.3087	0.8862	0.20
H(132)	4*a*		1.1361	0.4785	0.8927	0.20
C(14)	4*a*		1.142(5)	0.370(3)	0.9635(7)	0.16(1)
H(141)	4*a*		1.2848	0.3861	0.9694	0.20
H(142)	4*a*		1.1053	0.2734	0.9758	0.20
H(143)	4*a*		1.0644	0.4427	0.9823	0.20
C(20)	4*a*		0.269(2)	0.361(2)	0.6943(4)	0.079(5)
H(201)	4*a*		0.1914	0.2716	0.7010	0.20
H(202)	4*a*		0.1817	0.4438	0.7032	0.20
C(21)	4*a*		0.316(1)	0.368(2)	0.6362(4)	0.14(1)
H(211)	4*a*		0.4381	0.3108	0.6290	0.20
H(212)	4*a*		0.3436	0.4697	0.6263	0.20
C(22A)	4*a*	0.75	0.1422(8)	0.310(1)	0.6036(4)	0.18(1)
H(22A)	4*a*	0.75	0.1957	0.2589	0.5729	0.20
H(22A)	4*a*	0.75	0.0649	0.2392	0.6243	0.20
C(23A)	4*a*	0.75	0.003(5)	0.432(2)	0.586(1)	0.22(2)
H(23A)	4*a*	0.75	0.0844	0.5179	0.5764	0.20
H(23A)	4*a*	0.75	−0.0857	0.4603	0.6149	0.20
C(24)	4*a*		−0.124(3)	0.386(3)	0.5393(8)	0.22(2)
H(24A)	4*a*	0.75	−0.2100	0.4664	0.5287	0.20
H(24A)	4*a*	0.75	−0.2067	0.303	0.5489	0.20
H(24A)	4*a*	0.75	−0.0360	0.3592	0.5105	0.20
C(22B)	4*a*	0.25	0.1422(8)	0.310(1)	0.6036(4)	0.18
H(22B)	4*a*	0.25	0.1796	0.2149	0.5888	0.20
H(22B)	4*a*	0.25	0.0240	0.2954	0.6261	0.20
C(23B)	4*a*	0.25	0.088(5)	0.414(4)	0.560(1)	0.22
H(23B)	4*a*	0.25	0.1853	0.4028	0.5309	0.20
H(23B)	4*a*	0.25	0.0978	0.5151	0.5723	0.20
H(24B)	4*a*	0.25	−0.1555	0.4557	0.5120	0.20
H(24B)	4*a*	0.25	−0.2198	0.3966	0.5677	0.20
H(24B)	4*a*	0.25	−0.1317	0.2878	0.5253	0.20

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}
Sn(1)	4*a*	0.5271(1)	0.3634(1)	0.74548(5)	0.0362(5)	0.0496(6)	0.0994(8)	0.0031(4)	0.0006(5)	0.0025(7)
Cl(1)	4*a*	0.7318(6)	0.1672(4)	0.7118(2)	0.048(2)	0.048(2)	0.124(3)	0.002(2)	0.016(2)	−0.004(2)
Cl(2)	4*a*	0.7313(6)	0.5646(5)	0.7116(2)	0.044(2)	0.055(2)	0.130(4)	−0.005(2)	0.017(2)	0.005(3)

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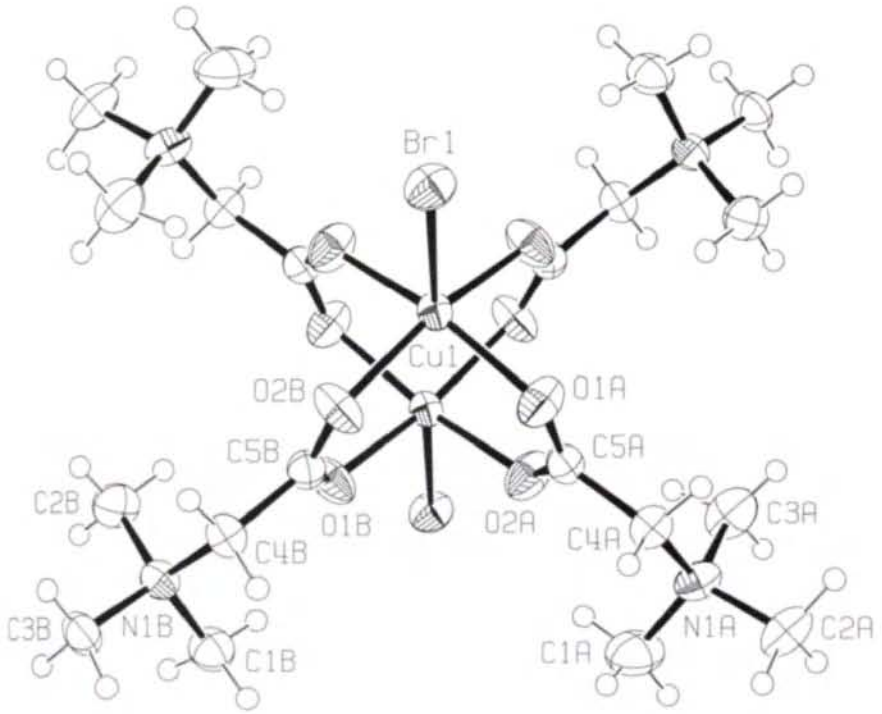

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