

Dichloridobis(2-chlorobenzyl)tin(IV)

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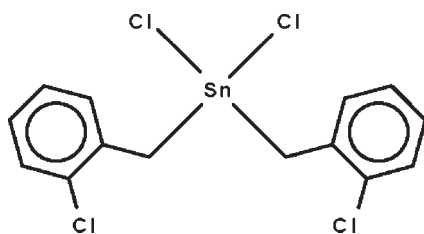
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.027; wR factor = 0.073; data-to-parameter ratio = 20.3.

Molecules of the title compound, $[\text{Sn}(\text{C}_7\text{H}_6\text{Cl})_2\text{Cl}_2]$, lie on a twofold rotation axis which passes through the Sn atom. The Sn^{IV} atom exists in a distorted tetrahedral geometry. Adjacent molecules are linked by weak $\text{Sn} \cdots \text{Cl}$ contacts [3.703 (1) Å], forming a linear chain motif extending along the b axis.

Related literature

For the synthesis of the title compound, see: Sisido *et al.* (1961). For the crystal structure of dichloridobis(2-fluorobenzyl)tin(IV), see: Yin & Gao (2006).



Experimental

Crystal data

$[\text{Sn}(\text{C}_7\text{H}_6\text{Cl})_2\text{Cl}_2]$

$M_r = 440.73$

Monoclinic, $C2/c$
 $a = 26.0750$ (13) Å
 $b = 4.7757$ (2) Å
 $c = 13.3389$ (7) Å
 $\beta = 112.1538$ (5)°
 $V = 1538.42$ (13) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.34$ mm⁻¹
 $T = 100$ K
 $0.40 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.455$, $T_{\text{max}} = 0.800$

8736 measured reflections
 1767 independent reflections
 1674 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.073$
 $S = 1.07$
 1767 reflections

87 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 2.12$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.03$ e Å⁻³

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5298).

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supplementary materials

Acta Cryst. (2010). E66, m966 [doi:10.1107/S1600536810028072]

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Comment

Diorganotin(IV) dichlorides have the tin centres in a tetrahedral environment but the coordination number can raise by tin–chlorine bridging; the bridging interaction can be regarded as a formal coordination bond if the distance is sufficiently short. In di(2-chlorobenzyl)tin dichloride (Scheme I, Fig. 1), as the interaction is 3.703 (1) Å, the geometry is better interpreted as being tetrahedral. The compound is isostructural with the fluorine analog (Yin & Gao, 2006).

Experimental

The compound was synthesized by the reaction of metallic tin with 2-benzyl chloride (Sisido *et al.*, 1961), and crystals were obtained by recrystallization from chloroform.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.95–0.99 Å) and included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. In the final difference Fourier map there is a peak ($2.122\text{e}/\text{Å}^3$) at 0.96 Å from Sn1 and a hole ($-1.027\text{e}/\text{Å}^3$) at 0.79 Å from Sn1.

Figures

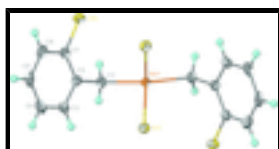


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $\text{SnCl}_2(\text{C}_7\text{H}_6\text{Cl})_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

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$M_r = 440.73$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 26.0750$ (13) Å

$b = 4.7757$ (2) Å

$c = 13.3389$ (7) Å

$\beta = 112.1538$ (5)°

$V = 1538.42$ (13) Å³

$F(000) = 856$

$D_x = 1.903$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7518 reflections

$\theta = 3.1$ – 28.3 °

$\mu = 2.34$ mm⁻¹

$T = 100$ K

Block, colorless

$0.40 \times 0.10 \times 0.10$ mm

supplementary materials

Z = 4

Data collection

Bruker SMART APEX diffractometer	1767 independent reflections
Radiation source: fine-focus sealed tube	1674 reflections with $I > 2\sigma(I)$
graphite	$R_{\text{int}} = 0.029$
ω scans	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -33 \rightarrow 33$
$T_{\text{min}} = 0.455$, $T_{\text{max}} = 0.800$	$k = -6 \rightarrow 6$
8736 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.073$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 6.0977P]$
1767 reflections	where $P = (F_o^2 + 2F_c^2)/3$
87 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 2.12 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -1.03 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	0.53623 (5)	0.7500	0.01430 (10)
Cl1	0.53371 (3)	0.85923 (15)	0.89559 (5)	0.02030 (16)
Cl2	0.33923 (3)	0.48153 (16)	0.55119 (6)	0.02400 (17)
C1	0.42929 (11)	0.3670 (6)	0.7750 (2)	0.0181 (5)
H1A	0.4121	0.2202	0.7202	0.022*
H1B	0.4417	0.2783	0.8473	0.022*
C2	0.38724 (11)	0.5857 (6)	0.7673 (2)	0.0161 (5)
C3	0.38871 (11)	0.7290 (6)	0.8594 (2)	0.0192 (5)
H3	0.4171	0.6866	0.9273	0.023*
C4	0.34985 (13)	0.9316 (7)	0.8546 (3)	0.0237 (6)
H4	0.3516	1.0249	0.9187	0.028*
C5	0.30839 (13)	0.9987 (6)	0.7564 (3)	0.0249 (6)
H5	0.2820	1.1390	0.7531	0.030*
C6	0.30554 (12)	0.8602 (7)	0.6627 (3)	0.0232 (6)
H6	0.2772	0.9050	0.5950	0.028*
C7	0.34455 (11)	0.6557 (6)	0.6692 (2)	0.0186 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01278 (15)	0.01420 (15)	0.01702 (15)	0.000	0.00688 (10)	0.000
Cl1	0.0189 (3)	0.0207 (4)	0.0207 (3)	-0.0001 (2)	0.0067 (2)	-0.0046 (2)
Cl2	0.0218 (3)	0.0308 (4)	0.0187 (3)	-0.0035 (3)	0.0068 (3)	-0.0029 (3)
C1	0.0158 (12)	0.0176 (13)	0.0233 (13)	0.0000 (10)	0.0100 (10)	0.0018 (10)
C2	0.0138 (12)	0.0148 (12)	0.0212 (13)	-0.0009 (9)	0.0084 (10)	0.0020 (10)
C3	0.0188 (12)	0.0217 (14)	0.0198 (13)	-0.0020 (10)	0.0104 (10)	0.0023 (11)
C4	0.0258 (15)	0.0219 (15)	0.0304 (15)	-0.0041 (11)	0.0185 (13)	-0.0043 (12)
C5	0.0184 (14)	0.0220 (14)	0.0406 (18)	0.0019 (10)	0.0182 (13)	0.0013 (12)
C6	0.0148 (12)	0.0244 (15)	0.0298 (15)	0.0001 (11)	0.0077 (11)	0.0055 (12)
C7	0.0162 (12)	0.0213 (14)	0.0205 (13)	-0.0025 (10)	0.0093 (10)	-0.0002 (10)

Geometric parameters (\AA , $^\circ$)

Sn1—C1 ⁱ	2.151 (3)	C2—C7	1.401 (4)
Sn1—C1	2.151 (3)	C3—C4	1.385 (4)
Sn1—Cl1	2.3740 (7)	C3—H3	0.9500
Sn1—Cl1 ⁱ	2.3740 (7)	C4—C5	1.385 (5)
Cl2—C7	1.739 (3)	C4—H4	0.9500
C1—C2	1.489 (4)	C5—C6	1.391 (5)
C1—H1A	0.9900	C5—H5	0.9500
C1—H1B	0.9900	C6—C7	1.389 (4)
C2—C3	1.395 (4)	C6—H6	0.9500
C1 ⁱ —Sn1—C1	135.86 (16)	C4—C3—C2	121.7 (3)
C1 ⁱ —Sn1—Cl1	107.23 (8)	C4—C3—H3	119.2
C1—Sn1—Cl1	101.07 (8)	C2—C3—H3	119.2
C1 ⁱ —Sn1—Cl1 ⁱ	101.07 (8)	C5—C4—C3	120.2 (3)
C1—Sn1—Cl1 ⁱ	107.23 (8)	C5—C4—H4	119.9
Cl1—Sn1—Cl1 ⁱ	98.96 (4)	C3—C4—H4	119.9
C2—C1—Sn1	112.17 (18)	C4—C5—C6	119.8 (3)
C2—C1—H1A	109.2	C4—C5—H5	120.1
Sn1—C1—H1A	109.2	C6—C5—H5	120.1
C2—C1—H1B	109.2	C7—C6—C5	119.2 (3)
Sn1—C1—H1B	109.2	C7—C6—H6	120.4
H1A—C1—H1B	107.9	C5—C6—H6	120.4
C3—C2—C7	117.0 (3)	C6—C7—C2	122.1 (3)
C3—C2—C1	120.5 (2)	C6—C7—Cl2	118.2 (2)
C7—C2—C1	122.5 (3)	C2—C7—Cl2	119.7 (2)

Symmetry codes: (i) $-x+1, y, -z+3/2$.

Fig. 1

