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Dibenzyldichloridotin(IV)

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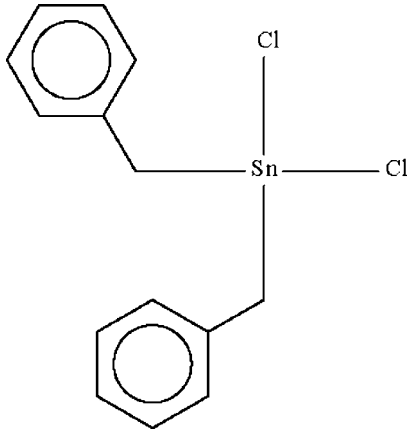
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.014; wR factor = 0.041; data-to-parameter ratio = 20.3.

The title compound, $[Sn(C_7H_7)_2Cl_2]$, exists as a monomeric tetrahedral molecule. The Sn atom lies on a special position of site symmetry 2. Adjacent molecules are linked into a linear chain running along the b axis of the monoclinic unit cell by Sn···Cl bridges of 3.7275 (4) Å.

Related literature

For the synthesis of dibenzyltin dichloride by the direct reaction of benzyl chloride and metallic tin, see: Shishido *et al.* (1961). For an overview of crystallographic and theoretical structures of diorganotin dichlorides, see: Buntine *et al.* (2003).



Experimental

Crystal data

$[Sn(C_7H_7)_2Cl_2]$
M_r = 371.84
Monoclinic, $C2/c$
a = 23.7710 (3) Å
b = 4.8019 (1) Å
c = 12.0808 (2) Å
β = 92.560 (1)°
V = 1377.60 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.22 mm^{-1}
T = 123 K
0.35 × 0.30 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.511, T_{max} = 0.732
6090 measured reflections
1580 independent reflections
1527 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.041
S = 1.03
1580 reflections
78 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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, 2009).

We thank the University of Malaya (FS339/2008A) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2438).

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supporting information

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S1. Experimental

Dibenzyltin dichloride was synthesized from benzyl chloride and metallic tin by a literature method (Shishido *et al.*, 1961). Crystals were obtained by recrystallization from chloroform.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95–0.99 Å) and were included in the refinement in the riding model approximation with *U*(H) set to 1.2*U*(C).

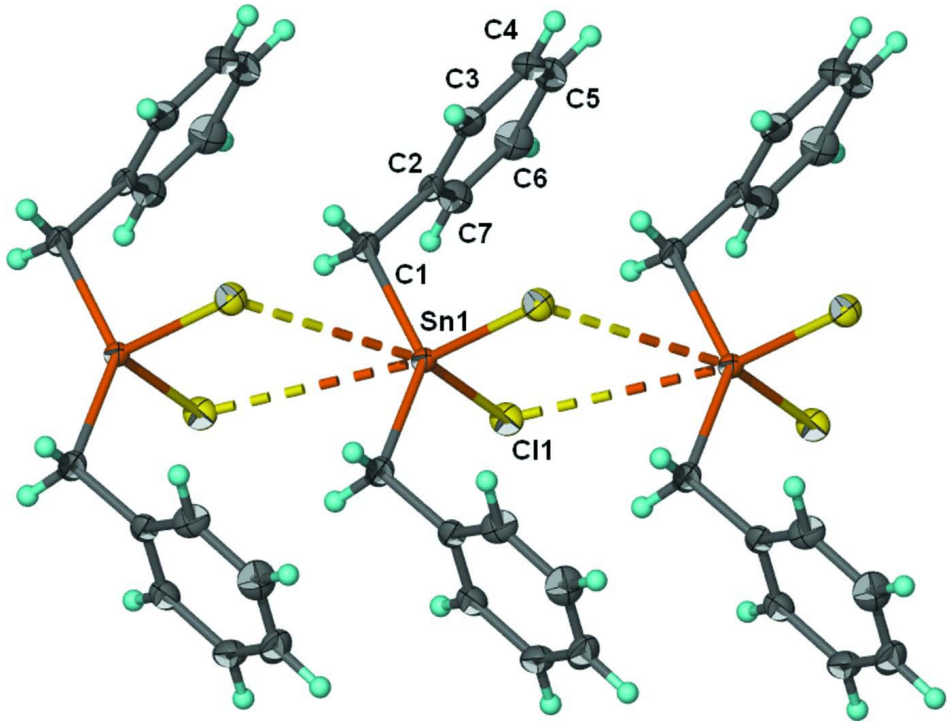

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of part of the supramolecular chain in $(C_6H_5CH_2)_2SnCl_2$ drawn at the 70% probability level. Dashed lines denote the Sn···Cl bridges. Hydrogen atoms are drawn as spheres of arbitrary radius. Unlabelled atoms within the partially labelled molecule are related by the symmetry operation: -x+1, y, -z+1/2.

Dibenzyldichloridotin(IV)

Crystal data

$[Sn(C_7H_7)_2Cl_2]$
$M_r = 371.84$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.7710\ (3)$ Å
$b = 4.8019\ (1)$ Å
$c = 12.0808\ (2)$ Å
$\beta = 92.560\ (1)°$
$V = 1377.60\ (4)$ Å^3
$Z = 4$
$F(000) = 728$
$D_x = 1.793$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5461 reflections
$\theta = 2.5–28.3°$
$\mu = 2.22$ mm^{-1}
$T = 123$ K
Block, colorless
0.35 × 0.30 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.511$, $T_{max} = 0.732$
6090 measured reflections
1580 independent reflections
1527 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$h = -30\rightarrow30$
$k = -6\rightarrow6$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.014$
$wR(F^2) = 0.041$
$S = 1.03$
1580 reflections
78 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 1.6061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.5000	0.49246 (2)	0.2500	0.01354 (6)
Cl1	0.473226 (16)	0.81293 (8)	0.38720 (3)	0.01976 (9)
C1	0.57846 (6)	0.3263 (3)	0.31462 (14)	0.0206 (3)
H1A	0.5716	0.2146	0.3816	0.025*
H1B	0.5942	0.2008	0.2588	0.025*
C2	0.62055 (7)	0.5502 (3)	0.34383 (14)	0.0175 (3)
C3	0.65796 (6)	0.6448 (3)	0.26657 (13)	0.0197 (3)
H3	0.6563	0.5694	0.1938	0.024*
C4	0.69765 (7)	0.8477 (3)	0.29468 (14)	0.0225 (3)
H4	0.7228	0.9111	0.2411	0.027*
C5	0.70071 (8)	0.9580 (3)	0.40082 (17)	0.0253 (4)
H5	0.7282	1.0952	0.4204	0.030*
C6	0.66358 (7)	0.8673 (4)	0.47815 (14)	0.0260 (3)

H6	0.6654	0.9436	0.5508	0.031*
C7	0.62366 (7)	0.6650 (3)	0.44994 (13)	0.0222 (3)
H7	0.5983	0.6044	0.5035	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01130 (9)	0.01254 (9)	0.01666 (9)	0.000	−0.00051 (6)	0.000
Cl1	0.02142 (18)	0.02114 (18)	0.01692 (16)	−0.00076 (14)	0.00309 (13)	−0.00308 (13)
C1	0.0153 (7)	0.0142 (7)	0.0318 (8)	0.0000 (6)	−0.0049 (6)	0.0023 (6)
C2	0.0129 (7)	0.0138 (6)	0.0254 (8)	0.0020 (6)	−0.0044 (6)	0.0025 (6)
C3	0.0168 (7)	0.0191 (7)	0.0232 (7)	0.0026 (6)	0.0001 (6)	−0.0025 (6)
C4	0.0145 (7)	0.0216 (7)	0.0316 (8)	−0.0003 (6)	0.0022 (6)	0.0026 (6)
C5	0.0195 (8)	0.0193 (7)	0.0361 (10)	−0.0029 (6)	−0.0081 (7)	−0.0010 (7)
C6	0.0271 (8)	0.0281 (8)	0.0222 (8)	0.0000 (7)	−0.0075 (6)	−0.0023 (6)
C7	0.0204 (8)	0.0249 (8)	0.0210 (7)	−0.0011 (6)	−0.0016 (6)	0.0051 (6)

Geometric parameters (Å, º)

Sn1—Cl1^{i}	3.7275 (4)	C3—C4	1.388 (2)
Sn1—C1^{ii}	2.143 (2)	C3—H3	0.9500
Sn1—C1	2.143 (2)	C4—C5	1.386 (3)
Sn1—Cl1	2.3695 (4)	C4—H4	0.9500
Sn1—Cl1^{ii}	2.3695 (4)	C5—C6	1.384 (3)
C1—C2	1.500 (2)	C5—H5	0.9500
C1—H1A	0.9900	C6—C7	1.390 (2)
C1—H1B	0.9900	C6—H6	0.9500
C2—C3	1.394 (2)	C7—H7	0.9500
C2—C7	1.394 (2)		
C1^{ii}—Sn1—C1	136.30 (8)	C4—C3—C2	120.80 (15)
C1^{ii}—Sn1—Cl1	103.88 (4)	C4—C3—H3	119.6
C1—Sn1—Cl1	104.09 (4)	C2—C3—H3	119.6
C1^{ii}—Sn1—Cl1^{ii}	104.09 (4)	C5—C4—C3	120.11 (15)
C1—Sn1—Cl1^{ii}	103.88 (4)	C5—C4—H4	119.9
Cl1—Sn1—Cl1^{ii}	99.001 (18)	C3—C4—H4	119.9
C2—C1—Sn1	112.29 (10)	C6—C5—C4	119.69 (16)
C2—C1—H1A	109.1	C6—C5—H5	120.2
Sn1—C1—H1A	109.1	C4—C5—H5	120.2
C2—C1—H1B	109.1	C5—C6—C7	120.24 (16)
Sn1—C1—H1B	109.1	C5—C6—H6	119.9
H1A—C1—H1B	107.9	C7—C6—H6	119.9
C3—C2—C7	118.52 (15)	C6—C7—C2	120.63 (15)
C3—C2—C1	120.99 (15)	C6—C7—H7	119.7
C7—C2—C1	120.48 (15)	C2—C7—H7	119.7
C1^{ii}—Sn1—C1—C2	177.45 (13)	C2—C3—C4—C5	0.4 (2)
Cl1—Sn1—C1—C2	−54.18 (12)	C3—C4—C5—C6	−0.8 (3)

Cl1^{ii}—Sn1—C1—C2	49.01 (12)	C4—C5—C6—C7	0.5 (3)
Sn1—C1—C2—C3	−90.75 (16)	C5—C6—C7—C2	0.2 (3)
Sn1—C1—C2—C7	90.34 (15)	C3—C2—C7—C6	−0.6 (2)
C7—C2—C3—C4	0.3 (2)	C1—C2—C7—C6	178.31 (15)
C1—C2—C3—C4	−178.60 (14)		

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