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An organotin coordination polymer formed from 1,4-bis(pyridin-3-ylmethoxy)benzene and dibenzyldichlorostannane

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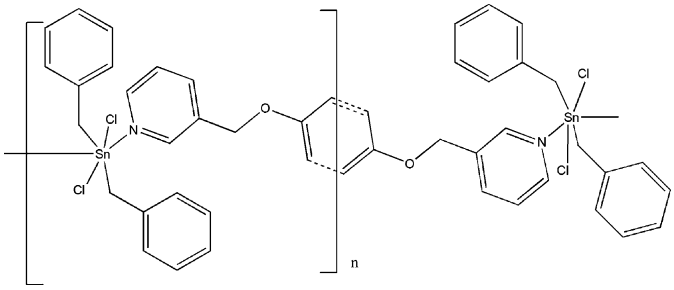
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.062; data-to-parameter ratio = 20.0.

In the title compound, *catena*-poly[[dibenzyldichloridotin(IV)]-μ-1,4-bis(pyridin-3-ylmethoxy)benzene], $[SnCl_2(C_7H_7)_2(C_{18}H_{16}N_2O_2)]_n$, the dibenzyldichlorostannane molecules are linked by the neutral 1,4-bis(pyridin-3-ylmethoxy)benzene ligands to generate an infinite coordination polymer. Both the Sn atom and the linking ligand reside on centers of inversion. The Sn atom displays a distorted octahedral geometry that consists of two benzyl groups, two chloride ions and two N atoms from different 1,4-bis(pyridin-3-ylmethoxy)benzene ligands.

Related literature

Metal-organic coordination polymers with aromatic *N*-donor ligands have attracted special attention owing to their interesting structural and chemical properties (Carlucci *et al.*, 2004; Cui *et al.*, 2005; Dobrzańska *et al.*, 2005). Aromatic *N*-donor ligands with different character have been selected for constructing new organotin compounds (Li *et al.*, 2006; Ma *et al.*, 2004). The Sn—N and Sn—Cl distances are in reported ranges (Pettinari *et al.*, 1998).



Experimental

Crystal data

$[SnCl_2(C_7H_7)_2(C_{18}H_{16}N_2O_2)]$
M_r = 664.17
Monoclinic, $P2_1/c$
a = 7.2380 (5) Å
b = 14.3560 (9) Å
c = 14.6290 (9) Å
β = 90.098 (1)°
V = 1520.08 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 293 (2) K
0.38 × 0.33 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.678, T_{max} = 0.746
9019 measured reflections
3558 independent reflections
3144 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 1.06
3558 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2174).

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supplementary materials

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An organotin coordination polymer formed from 1,4-bis(pyridin-3-ylmethoxy)benzene and dibenzyldichlorostannane

S.-L. Li, J. Liu and J.-F. Ma

Comment

In recent years, metal-organic coordination polymers with aromatic N-donor ligands have attracted special attention owing to their interesting structural and chemical properties (Carlucci *et al.*, 2004; Cui *et al*., 2005; Dobrzańska *et al.*, 2005). Aromatic N-donor ligands with different character are selected for constructing new compounds with organotin (Li *et al.*, 2006; Ma *et al.*, 2004). In this case, 1,4-bis(pyridin-3-ylmethoxy)benzene and dibenzyldichlorostannane were selected to construct complexes with a polymeric structure.

In the title compound, $\{(C_7H_7)_2SnCl_2(C_{18}H_{16}O_2N_2)\}_n$, the asymmetric unit contains one Sn(IV) atom located on a center of inversion. As shown in Figure 1, the Sn has a distorted octahedral coordination geometry that consists of two benzyl groups,two Cl^- ions and two nitrogen atoms from different 1,4-bis(pyridin-3-ylmethoxy)benzene ligands. All the distances of Sn—N and Sn—Cl are in the reported ranges (Pettinari *et al.*, 1998). In addition, the dihedral angle of the phenyl ring and pyridine ring is 49.5 (4)°. Each dibenzyldichlorostannane is linked by the neutral 1,4-bis(pyridin-3-ylmethoxy)benzene ligands to generate an infinite coordination polymeric chain, and all chains are parallel in the structure.

Experimental

A mixture of hydroquinone (1.0 g, 10 mmol) and NaOH (0.8 g, 20 mmol) in DMSO (20 ml) was stirred at 60°C for 1 h, then 3-(chloromethyl)pyridine (2.6 g, 20 mmol) was added. The mixture was cooled to room temperature after stirring at 60°C for 24 h, and then poured into 100 ml of water. A colorless solid of 1,4-bis(pyridin-3-ylmethoxy)benzene formed immediately, which was isolated by filtration in 68% yield after drying in air.

A mixture of dibenzyldichlorostannane (37 mg, 0.1 mmol) (obtained from commercial sources) with 1,4-bis(pyridin-3-ylmethoxy)benzene (29 mg, 0.1 mmol) in EtOH and CH_2Cl_2 (25 ml, v:v = 1:1) was stirred for a few minutes and then filtered. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the filtrate at room temperature for several days (yield: 35%). Analysis calculated for $C_{32}H_{30}Cl_2N_2O_2Sn$: C 57.86, H 4.55, N 4.22%; found: C 57.82, H 4.59, N 4.19%.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å for aromatic hydrogen atoms and C—H = 0.97 Å for methylene hydrogen atoms, and U_{iso}=1.2U_{eq}(C).

Figures

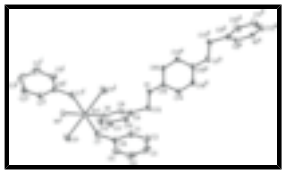


Fig. 1. A view of the molecule of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (i) = 1 − *x*, 1 − *y*, 1 − *z*; (ii) = 2 − *x*, 1 − *y*, −*z*.

catena-poly[[dibenzyldichloridotin(IV)]-μ-1,4-bis(pyridin-3-ylmethoxy)benzene]

Crystal data

$[SnCl_2(C_7H_7)_2(C_{18}H_{16}N_2O_2)]$	$Z = 2$
$M_r = 664.17$	$F_{000} = 672$
Monoclinic, $P2_1/c$	$D_x = 1.451$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 7.2380$ (5) Å	$\theta = 2.0$–28.5º
$b = 14.3560$ (9) Å	$\mu = 1.05$ mm^{-1}
$c = 14.6290$ (9) Å	$T = 293$ (2) K
$\beta = 90.098$ (1)º	Block, colorless
$V = 1520.08$ (17) Å^3	0.38 × 0.33 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer	3558 independent reflections
Radiation source: fine-focus sealed tube	3144 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 293$(2) K	$\theta_{max} = 28.5$º
ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -5 \rightarrow 9$
$T_{min} = 0.678$, $T_{max} = 0.746$	$k = -18 \rightarrow 18$
9019 measured reflections	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 0.426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3558 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}

178 parameters	$\Delta\rho_{min} = -0.80$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.5000	0.5000	0.5000	0.03137 (6)
Cl1	0.20749 (7)	0.43159 (4)	0.57024 (3)	0.05319 (13)
C1	0.8020 (3)	0.29921 (14)	0.38280 (14)	0.0532 (5)
H1	0.9066	0.3322	0.4006	0.064*
C2	0.8068 (5)	0.24379 (18)	0.30446 (18)	0.0773 (9)
H2	0.9140	0.2404	0.2697	0.093*
C3	0.6534 (6)	0.19451 (18)	0.27899 (18)	0.0898 (11)
H3	0.6568	0.1576	0.2268	0.108*
C4	0.4961 (5)	0.19903 (18)	0.3293 (2)	0.0842 (9)
H4	0.3929	0.1650	0.3113	0.101*
C5	0.4881 (4)	0.25374 (15)	0.40689 (17)	0.0596 (6)
H5	0.3798	0.2562	0.4409	0.072*
C6	0.6417 (3)	0.30517 (12)	0.43423 (12)	0.0415 (4)
C7	0.6336 (3)	0.36578 (13)	0.51685 (13)	0.0450 (4)
H7A	0.7589	0.3765	0.5380	0.054*
H7B	0.5694	0.3320	0.5646	0.054*
C8	0.5061 (2)	0.45295 (11)	0.28016 (10)	0.0322 (3)
H8	0.6321	0.4607	0.2901	0.039*
C9	0.4468 (2)	0.42783 (12)	0.19347 (11)	0.0346 (3)
C10	0.2592 (3)	0.41791 (16)	0.17951 (13)	0.0507 (5)
H10	0.2141	0.4004	0.1225	0.061*
C11	0.1393 (3)	0.43422 (18)	0.25106 (13)	0.0556 (6)
H11	0.0124	0.4293	0.2423	0.067*
C12	0.2089 (2)	0.45780 (15)	0.33514 (12)	0.0429 (4)
H12	0.1274	0.4680	0.3832	0.051*
C13	0.5846 (3)	0.41269 (13)	0.11814 (12)	0.0410 (4)
H13A	0.6507	0.3547	0.1276	0.049*
H13B	0.5223	0.4098	0.0595	0.049*
C14	0.8871 (3)	0.42179 (13)	−0.00519 (12)	0.0436 (4)
H14	0.8118	0.3695	−0.0092	0.052*

C15	0.8503 (3)	0.49061 (12)	0.05819 (13)	0.0396 (4)
C16	0.9622 (3)	0.56830 (14)	0.06280 (13)	0.0460 (4)
H16	0.9362	0.6147	0.1052	0.055*
O1	0.7078 (2)	0.48820 (10)	0.12015 (12)	0.0590 (5)
N1	0.39040 (19)	0.46651 (11)	0.35020 (9)	0.0328 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02965 (9)	0.03914 (10)	0.02533 (9)	0.00382 (6)	0.00442 (6)	−0.00170 (5)
Cl1	0.0395 (2)	0.0754 (3)	0.0447 (3)	−0.0091 (2)	0.00994 (19)	−0.0005 (2)
C1	0.0660 (13)	0.0428 (10)	0.0509 (12)	0.0122 (9)	0.0140 (10)	0.0053 (9)
C2	0.125 (2)	0.0526 (13)	0.0544 (14)	0.0342 (15)	0.0313 (15)	0.0074 (11)
C3	0.180 (4)	0.0434 (13)	0.0463 (14)	0.0161 (17)	−0.0108 (18)	−0.0093 (10)
C4	0.129 (3)	0.0485 (14)	0.0748 (18)	−0.0162 (15)	−0.0235 (18)	−0.0062 (12)
C5	0.0737 (15)	0.0441 (11)	0.0610 (13)	−0.0067 (10)	−0.0047 (11)	0.0067 (9)
C6	0.0542 (11)	0.0330 (8)	0.0373 (9)	0.0084 (8)	0.0019 (8)	0.0047 (7)
C7	0.0515 (11)	0.0466 (10)	0.0368 (9)	0.0134 (8)	−0.0011 (8)	0.0007 (8)
C8	0.0274 (7)	0.0404 (9)	0.0290 (8)	−0.0003 (6)	0.0033 (6)	0.0018 (6)
C9	0.0352 (8)	0.0431 (9)	0.0255 (7)	−0.0043 (7)	0.0064 (6)	0.0024 (6)
C10	0.0404 (10)	0.0822 (15)	0.0296 (9)	−0.0124 (10)	−0.0009 (7)	−0.0004 (9)
C11	0.0296 (9)	0.1006 (18)	0.0367 (10)	−0.0086 (10)	0.0001 (7)	0.0035 (10)
C12	0.0300 (8)	0.0652 (12)	0.0334 (9)	0.0003 (8)	0.0067 (7)	0.0024 (8)
C13	0.0430 (9)	0.0498 (10)	0.0303 (8)	−0.0100 (8)	0.0094 (7)	−0.0059 (7)
C14	0.0444 (10)	0.0481 (10)	0.0383 (9)	−0.0156 (8)	0.0119 (7)	−0.0131 (8)
C15	0.0380 (9)	0.0495 (10)	0.0313 (9)	−0.0067 (7)	0.0113 (7)	−0.0080 (7)
C16	0.0466 (10)	0.0505 (10)	0.0410 (10)	−0.0130 (8)	0.0171 (8)	−0.0188 (8)
O1	0.0566 (9)	0.0633 (9)	0.0572 (10)	−0.0258 (7)	0.0344 (8)	−0.0252 (7)
N1	0.0302 (7)	0.0419 (7)	0.0263 (7)	0.0009 (6)	0.0031 (5)	0.0013 (6)

Geometric parameters (Å, °)

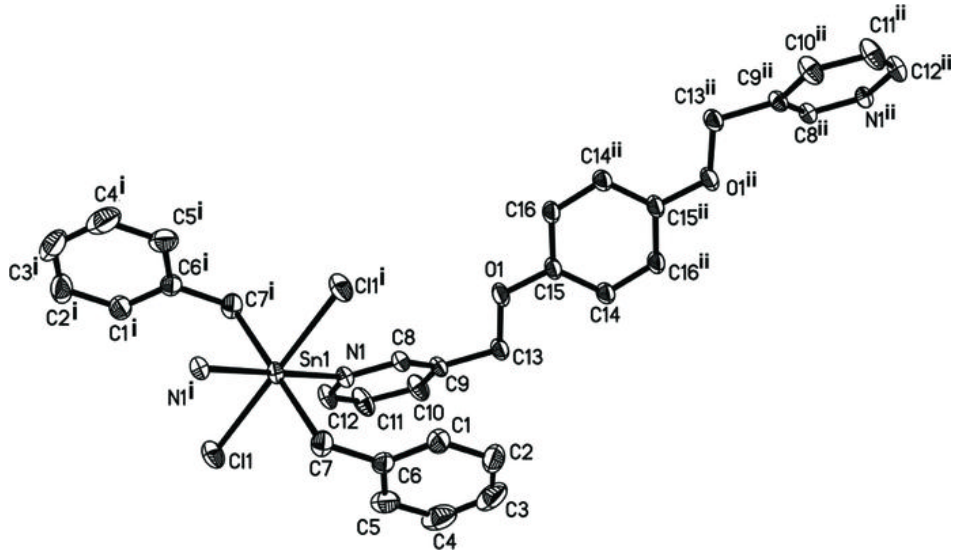
Sn1—C7	2.1696 (18)	C8—H8	0.9300
Sn1—N1	2.3784 (14)	C9—C10	1.380 (2)
Sn1—Cl1	2.5515 (5)	C9—C13	1.504 (2)
C1—C6	1.387 (3)	C10—C11	1.381 (3)
C1—C2	1.396 (3)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.371 (3)
C2—C3	1.368 (5)	C11—H11	0.9300
C2—H2	0.9300	C12—N1	1.338 (2)
C3—C4	1.358 (5)	C12—H12	0.9300
C3—H3	0.9300	C13—O1	1.404 (2)
C4—C5	1.382 (4)	C13—H13A	0.9700
C4—H4	0.9300	C13—H13B	0.9700
C5—C6	1.393 (3)	C14—C15	1.381 (2)
C5—H5	0.9300	C14—C16^{i}	1.387 (2)
C6—C7	1.491 (3)	C14—H14	0.9300
C7—H7A	0.9700	C15—O1	1.375 (2)

C7—H7B	0.9700	C15—C16	1.380 (3)
C8—N1	1.339 (2)	C16—C14^{i}	1.387 (2)
C8—C9	1.386 (2)	C16—H16	0.9300
C7—Sn1—N1	94.19 (6)	C10—C9—C13	122.04 (15)
C7—Sn1—Cl1	88.98 (6)	C8—C9—C13	120.23 (15)
N1—Sn1—Cl1	91.01 (4)	C9—C10—C11	119.34 (17)
C6—C1—C2	120.2 (2)	C9—C10—H10	120.3
C6—C1—H1	119.9	C11—C10—H10	120.3
C2—C1—H1	119.9	C12—C11—C10	119.43 (17)
C3—C2—C1	119.8 (3)	C12—C11—H11	120.3
C3—C2—H2	120.1	C10—C11—H11	120.3
C1—C2—H2	120.1	N1—C12—C11	122.02 (16)
C4—C3—C2	120.6 (2)	N1—C12—H12	119.0
C4—C3—H3	119.7	C11—C12—H12	119.0
C2—C3—H3	119.7	O1—C13—C9	107.17 (14)
C3—C4—C5	120.6 (3)	O1—C13—H13A	110.3
C3—C4—H4	119.7	C9—C13—H13A	110.3
C5—C4—H4	119.7	O1—C13—H13B	110.3
C4—C5—C6	120.2 (3)	C9—C13—H13B	110.3
C4—C5—H5	119.9	H13A—C13—H13B	108.5
C6—C5—H5	119.9	C15—C14—C16^{i}	119.17 (17)
C1—C6—C5	118.7 (2)	C15—C14—H14	120.4
C1—C6—C7	120.68 (19)	C16^{i}—C14—H14	120.4
C5—C6—C7	120.66 (19)	O1—C15—C16	115.42 (15)
C6—C7—Sn1	116.39 (12)	O1—C15—C14	124.78 (16)
C6—C7—H7A	108.2	C16—C15—C14	119.80 (17)
Sn1—C7—H7A	108.2	C15—C16—C14^{i}	121.03 (16)
C6—C7—H7B	108.2	C15—C16—H16	119.5
Sn1—C7—H7B	108.2	C14^{i}—C16—H16	119.5
H7A—C7—H7B	107.3	C15—O1—C13	118.87 (14)
N1—C8—C9	123.04 (15)	C12—N1—C8	118.41 (14)
N1—C8—H8	118.5	C12—N1—Sn1	119.77 (11)
C9—C8—H8	118.5	C8—N1—Sn1	121.78 (11)
C10—C9—C8	117.73 (15)		
C6—C1—C2—C3	−0.7 (3)	C8—C9—C13—O1	−46.9 (2)
C1—C2—C3—C4	0.0 (4)	C16^{i}—C14—C15—O1	−178.7 (2)
C2—C3—C4—C5	0.2 (4)	C16^{i}—C14—C15—C16	0.6 (3)
C3—C4—C5—C6	0.2 (4)	O1—C15—C16—C14^{i}	178.7 (2)
C2—C1—C6—C5	1.1 (3)	C14—C15—C16—C14^{i}	−0.6 (4)
C2—C1—C6—C7	−178.63 (18)	C16—C15—O1—C13	178.23 (19)
C4—C5—C6—C1	−0.8 (3)	C14—C15—O1—C13	−2.5 (3)
C4—C5—C6—C7	178.9 (2)	C9—C13—O1—C15	179.19 (18)
C1—C6—C7—Sn1	100.43 (18)	C11—C12—N1—C8	1.0 (3)
C5—C6—C7—Sn1	−79.3 (2)	C11—C12—N1—Sn1	−176.86 (17)
N1^{ii}—Sn1—C7—C6	−171.71 (16)	C9—C8—N1—C12	−1.8 (3)
N1—Sn1—C7—C6	8.29 (16)	C9—C8—N1—Sn1	175.98 (13)

$Cl1^{ii}$—Sn1—C7—C6	−80.77 (15)	C7—Sn1—N1—C12	112.89 (15)
Cl1—Sn1—C7—C6	99.23 (15)	$C7^{ii}$—Sn1—N1—C12	−67.11 (15)
N1—C8—C9—C10	0.9 (3)	$Cl1^{ii}$—Sn1—N1—C12	−156.17 (14)
N1—C8—C9—C13	−179.33 (16)	Cl1—Sn1—N1—C12	23.83 (14)
C8—C9—C10—C11	0.8 (3)	C7—Sn1—N1—C8	−64.88 (14)
C13—C9—C10—C11	−179.0 (2)	$C7^{ii}$—Sn1—N1—C8	115.12 (14)
C9—C10—C11—C12	−1.5 (4)	$Cl1^{ii}$—Sn1—N1—C8	26.06 (13)
C10—C11—C12—N1	0.7 (4)	Cl1—Sn1—N1—C8	−153.94 (13)
C10—C9—C13—O1	132.9 (2)		

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C4i
C5i
C3i
C6i
C7i
Cl1i
C2i
C1i
Sn1
N1
C8
C13
O1
C15
C14
C16
C15ii
C16ii
O1ii
C14ii
C13ii
C9ii
C10ii
C11ii
C12ii
N1ii
C8ii
N1i
C9
C12
C11
C10
C1
C2
Cl1
C7
C6
C3
C5
C4