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catena-Poly[*fac*-trichloromethyltin(IV)-μ-[*meso*-1,2-bis(phenylsulfinyl)ethane-*O*:*O*′]]

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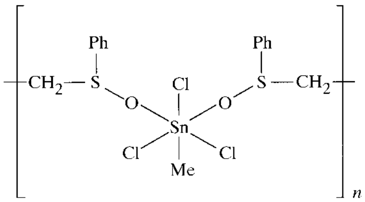
In the title compound, $[SnCl_3(CH_3)(C_6H_5SOCH_2)_2]_n$, the octahedral Sn^{IV} centres are bridged by *meso*-1,2-bis(phenylsulfinyl)ethane ligands forming infinite chains along the [100] direction.

Comment

This study is part of structural studies on adducts of halide–organotin compounds with sulfoxide derivatives.

The *meso*-1,2-bis(phenylsulfinyl)ethane ligand, *meso*-$(C_6H_5SOCH_2)_2$, crystallizes with a centre of symmetry at the middle of the ethane C—C bond (Cattalini *et al.*, 1979). The occurrence of this centre of symmetry was also observed here, (I), and in the structures of $[SnCl_2(CH_3)_2\{$*meso*-$(C_6H_5SOCH_2)_2\}]$ (Carvalho *et al.*, 1996*a*), $[SnCl_2(CH_3)_2\{$*meso*-$(C_3H_7SOCH_2)_2\}]$ (Carvalho *et al.*, 1996*b*) and *cis*-$[PtCl_2\{P(C_2H_5)_3\}\{$*meso*-$(C_6H_5SOCH_2)_2\}]_2$ (Francisco *et al.*, 1995), where the Sn^{IV} and Pt^{II} cations have octahedral and square-planar geometries, respectively.



(I)

In the title structure, the Sn^{IV} atom is hexacoordinate in a distorted octahedral geometry. The Cl atoms *trans* to the O atoms form Sn—Cl bonds [Sn—Cl2 2.4585 (8) and Sn—Cl3 2.4401 (8) Å] longer than the Cl atom *trans* to the C atom [Sn—Cl1 2.3774 (9) Å]. Completing the coordination, there are two equivalent sulfoxide groups in a *cis* orientation [both with an Sn—O distance of 2.227 (2) Å] and a methyl group at a Sn—C distance of 2.114 (3) Å. Each sulfoxide is bound to two Sn atoms in an infinite chain along the [100] direction.

Similar *cis*-O_2Sn geometries have been observed previously in the structures of $[SnCl_2(CH_3)_2\{$*meso*-$(C_6H_5SOCH_2)_2\}]$ and $[SnCl_2(CH_3)_2\{$*meso*-$(C_3H_7SOCH_2)_2\}]$. The average Sn—O bond distances (2.359 Å) in these structures compared with Sn—O [2.227 (2) Å] in the title complex, follow the expected trends in the lower Lewis acidity of $(CH_3)_2SnCl_2$ with respect to CH_3SnCl_3.

The crystal structures of the related adducts *mer*-$[SnCl_3(CH_3)(C_5H_4NSOC_3H_7)]$ (Sousa *et al.*, 1992), *fac*-$[SnCl_3\{(C_6H_5)CH_2\}(C_{12}H_8N_2)]$ (Hall & Tiekink, 1996) and *fac*- and *mer*-$[SnCl_3(C_3H_7)(C_4H_7NO)_2]$ (Reuter & Puff, 1992) have been determined. All these examples, and also the results observed for the title compound, agree with the proposal of Reuter & Puff (1992) that the predominant formation of only a special stereoisomer, which is often observed in octahedral 1:1 and/or 1:2 adducts of monoorganotin trihalides, is caused by reaction conditions more than steric and/or electronic effects of the several complex ligands.

Experimental

Suitable single crystals of (I) were obtained by the 1:1 reaction of *meso*-$(C_6H_5SOCH_2)_2$ with CH_3SnCl_3 in CH_2Cl_2.

Crystal data

$[SnCl_3(CH_3)(C_7H_7OS)_2]$
$M_r = 518.45$
Monoclinic, $P2_1/c$
$a = 15.942\ (1)$ Å
$b = 6.3738\ (4)$ Å
$c = 20.895\ (2)$ Å
$\beta = 111.129\ (7)^\circ$
$V = 1980.4\ (3)$ Å^3
$Z = 4$

$D_x = 1.739$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.34$–18.11°
$\mu = 1.91$ mm^{-1}
$T = 293\ (2)$ K
Prism, white
0.30 × 0.15 × 0.15 mm

Data collection

Enraf–Nonius Turbo–CAD-4 diffractometer
κ-geometry diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.670$, $T_{max} = 0.762$
5933 measured reflections
5748 independent reflections

4177 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 29.99^\circ$
$h = -22 \rightarrow 0$
$k = 0 \rightarrow 8$
$l = -27 \rightarrow 29$
3 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

Refinement on F^2
$R(F) = 0.031$
$wR(F^2) = 0.087$
$S = 1.054$
5748 reflections
210 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.0144P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0017 (2)

Table 1
Selected geometric parameters (Å, °).

Sn—C	2.114 (3)	S1—C1	1.779 (3)
Sn—O2	2.227 (2)	S1—C13	1.803 (3)
Sn—O1	2.227 (2)	S2—O2	1.532 (2)
Sn—Cl1	2.3774 (9)	S2—C7	1.782 (3)
Sn—Cl3	2.4401 (8)	S2—C14	1.804 (3)
Sn—Cl2	2.4585 (8)	C13—C13^{i}	1.511 (6)
S1—O1	1.535 (2)	C14—C14^{ii}	1.511 (6)
C—Sn—O2	86.89 (11)	O1—Sn—Cl2	87.42 (6)
C—Sn—O1	86.56 (11)	Cl1—Sn—Cl2	90.31 (3)
O2—Sn—O1	85.47 (8)	Cl3—Sn—Cl2	96.75 (3)
C—Sn—Cl1	167.70 (10)	O1—S1—C1	104.02 (13)
O2—Sn—Cl1	85.14 (6)	O1—S1—C13	103.59 (12)
O1—Sn—Cl1	83.49 (6)	C1—S1—C13	100.96 (14)
C—Sn—Cl3	97.55 (10)	O2—S2—C7	103.54 (14)
O2—Sn—Cl3	90.04 (6)	O2—S2—C14	104.26 (13)
O1—Sn—Cl3	173.76 (6)	C7—S2—C14	99.03 (14)
Cl1—Sn—Cl3	91.82 (4)	S1—O1—Sn	121.86 (12)
C—Sn—Cl2	96.46 (10)	S2—O2—Sn	126.83 (13)
O2—Sn—Cl2	171.95 (6)		

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

H atoms were positioned geometrically and a riding model was used during the refinement process, with U_{iso} amounting to 1.5 (for methyl H atoms) or 1.2 (for the remaining) of the value of the U_{eq} of the atom to which they are attached. The C—H distances range is 0.93–0.97 Å.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1998).

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