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cis-trans-Tetrachlorobis(dimethyl sulfide-κS)tin

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(S–C) = 0.002 Å
R factor = 0.018
wR factor = 0.041
Data-to-parameter ratio = 32.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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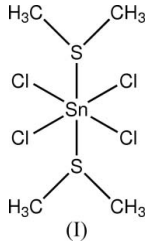
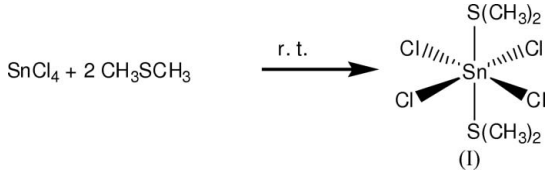
The molecule of the title compound, $[SnCl_4(C_2H_6S)_2]$, is located on a centre of inversion with a half-molecule in the asymmetric unit. The Sn atom shows a quadratic bipyramidal coordination.

Comment

Recently, we have reported on the synthesis and structure of the adduct of Me_3SnCl with Me_3SnOH and H_2O. This adduct represents an intermediate in Me_3SnCl hydrolysis. The structure of $Me_3SnCl{\cdot}Me_3SnOH{\cdot}H_2O$ features an array of Me_3Sn units connected alternately by bridging Cl and OH ligands (Lerner *et al.*, 2005). We report here the X-ray crystal structure analysis of the adduct $[SnCl_4]{\cdot}[CH_3SCH_3]_2$, (I). The synthesis of (I) was achieved by treatment of $SnCl_4$ with 2 equivalents of CH_3SCH_3, as indicated in the scheme below.



(I)



(I)

A perspective view of (I) is shown in Fig. 1 and a packing diagram is shown in Fig. 2. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.7 plus three updates; Allen, 2002). The coordination mode of the Sn atom is almost perfect quadratic bipyramidal. The two dimethyl sulfide residues occupy the apical positions and the Cl ligands are located in the quadratic plane. One Cl ligand almost bisects the $CH_3{-}S{-}CH_3$ angle (Table 1).

It is remarkable that *cis-trans*-tetrabromo-bis(dimethylthio)tin, (II) (Bricklebank *et al.*, 1994), is not isostructural with the title compound. Nevertheless, the cell parameters show some similarities: after transforming the cell of (II) from $P2_1/c$ into $P2_1/n$, the cell parameters are: a = 7.617 Å, b = 12.382 Å, c = 23.209 Å and β = 102.98°. Unfortunately, no coordinates are available for (II). Therefore, the two structures cannot be compared.

Experimental

$SnCl_4$ (0.71 ml) was added with stirring at ambient temperature to CH_3SCH_3 (25 ml). Colourless crystals of the title compound were grown by storing this solution at room temperature for several days.

Crystal data

$[SnCl_4(C_2H_6S)_2]$
M_r = 384.75
Monoclinic, $P2_1/n$
a = 6.6711 (5) Å
b = 12.2317 (8) Å
c = 8.1051 (6) Å
β = 107.068 (6)°
V = 632.24 (8) Å^3
Z = 2
D_x = 2.021 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15669 reflections
θ = 3.5–29.9°
μ = 3.14 mm^{-1}
T = 173 (2) K
Block, colourless
0.10 × 0.07 × 0.04 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.744, T_{max} = 0.885
15669 measured reflections
1798 independent reflections
1673 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 29.7°
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.042
S = 1.13
1798 reflections
55 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 0.192P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0191 (10)

Table 1
Selected geometric parameters (Å, °).

Sn1—Cl2	2.4147 (4)	Sn1—S1	2.6208 (4)
Sn1—Cl1	2.4188 (5)		
Cl2—Sn1—Cl1^i	89.669 (17)	Cl1—Sn1—S1	89.120 (14)
Cl2—Sn1—Cl1	90.332 (17)	C1—S1—C2	99.84 (9)
Cl2—Sn1—S1	91.174 (14)		
Cl1^i—Sn1—S1—C1	56.15 (7)	Cl1^i—Sn1—S1—C2	−47.87 (7)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

H atoms were located in a difference map and refined with fixed individual displacement parameters [U_{iso}(H) = 1.5U_{eq}(C)], using a riding model, with C—H = 0.98 Å. The methyl groups were allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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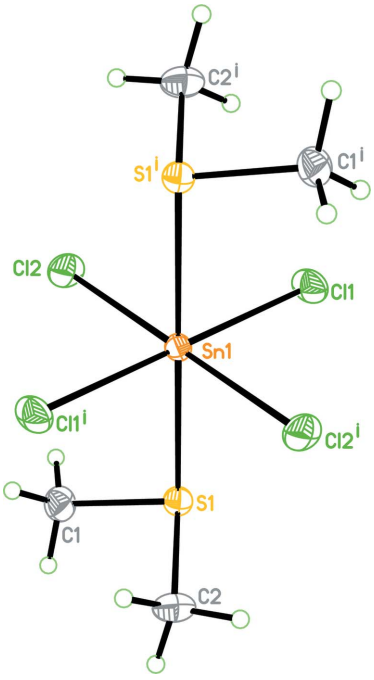

Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level for non-H atoms. [Symmetry code: (i) $-x+1, -y+1, -z+1$.]

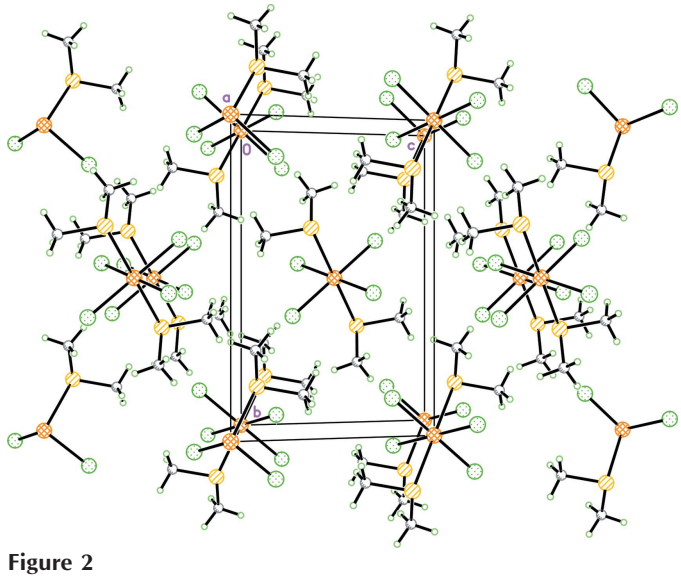

Figure 2
The packing of the title compound, viewed along the *a* axis.

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