

Edward R. T. Tiekink,\* James L. Wardell\* and William B. Welte

Department of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA

Correspondence e-mail:  
edward.tiekink@utsa.edu, che415@abdn.ac.uk,  
che415@abdn.ac.uk

## Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.021  
 $wR$  factor = 0.057  
Data-to-parameter ratio = 23.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dichloro(*N,N'*-diethyldithiocarbamato- $\kappa^2\text{S,S}'$ )-(4-methylpentan-2-onato- $\kappa^2\text{C}^4,\text{O}$ )tin(IV)

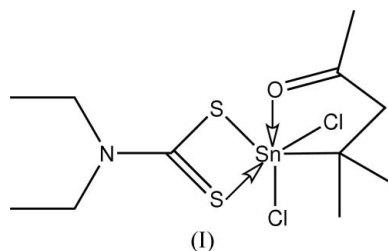
The title compound,  $[\text{SnCl}_2(\text{C}_5\text{H}_{10}\text{NS}_2)(\text{C}_6\text{H}_{11}\text{O})]$ , features an octahedrally coordinated Sn center within a  $\text{CCl}_2\text{OS}_2$  donor set defined by chelating dithiocarbamate and 4-methylpentan-2-onate ligands and *cis*-Cl atoms. The crystal structure comprises layers of molecules interconnected by  $\text{C}-\text{H}\cdots\text{Cl}$  interactions.

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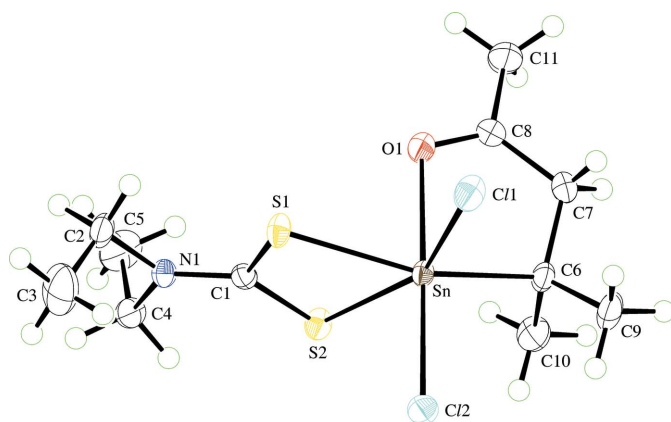
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## Comment

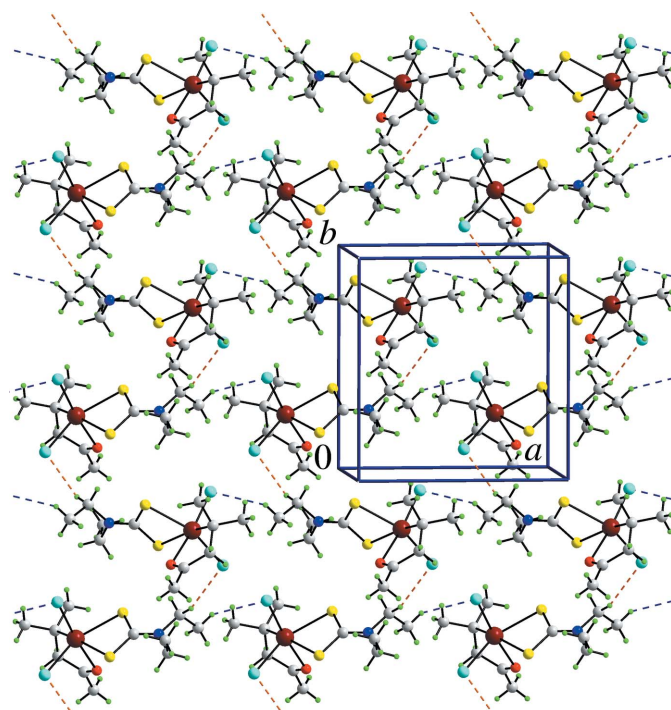
Organotin dithiocarbamate compounds related to the title compound, (I), continue to attract interest owing to their utility as single-source precursors for Chemical Vapor Deposition (CVD) of SnS (*e.g.*, Menezes *et al.*, 2004), as putative pharmaceuticals (*e.g.*, Donoghue *et al.*, 1993), and their structural diversity (Tiekink, 1992). The Sn atom in (I) (Fig. 1) displays a distorted octahedral geometry defined by two S atoms, derived from an asymmetrically chelating dithiocarbamate ligand, C- and O-donor atoms from a chelating 4-methylpentan-2-onate ligand and two terminal and *cis*-Cl atoms. The disparity in the Sn—S bond distances (Table 1) is reflected in both the magnitude of the C—S distances, *i.e.* long Sn—S2 is associated with short C1—S2, as well as in the Sn—Cl distances. Thus, the longer Sn—Cl1 distance involves the Cl1 atom that is approximately *trans* to S1 as opposed to the shorter Sn—Cl2 distance with Cl2 opposite to the Sn—O<sub>carbonyl</sub> bond. While the SnS<sub>2</sub>C chelate ring is effectively planar, there is significant puckering in the five-membered ring, as seen in the magnitudes of the Sn—C6—C7—C8 and O1—C8—C7—C6 torsion angles of 24.6 (3) and  $-32.7$  (2)°, respectively; these two rings are approximately orthogonal.



Molecules of (I) associate *via*  $\text{C}-\text{H}\cdots\text{Cl}$  interactions, forming a layer structure as shown in Fig. 2. A methylene and a methyl H atom of one ethyl group each forms such an interaction with two symmetry-related Cl atoms, displaced laterally, so that each molecule is involved in four such hydrogen-bonding interactions. Referring to Fig. 2, the C5—H $\cdots$ Cl1 contacts, highlighted as blue dashed lines, link mol-



**Figure 1**  
The molecular structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
The layer structure in (I) mediated by C—H...Cl interactions, shown as dashed lines. Color code: Sn brown, Cl cyan, S yellow, O red, N blue, C grey and H green.

ecules into chains along the *a*-axis direction; H...Cl<sup>ii</sup> is 2.81 Å, C5...Cl<sup>ii</sup> is 3.697 (3) Å and the angle at H is 150° [symmetry code: (i) 1 + *x*, *y*, *z*]. These chains are interconnected by C4—H...Cl<sup>iii</sup> contacts, shown as orange dashed lines along the *b*-axis direction, so that H...Cl<sup>iii</sup> is 2.80 Å, C4...Cl<sup>iii</sup> is 3.654 (2) Å and the angle at H is 145° [symmetry code: (ii) 2 - *x*,  $\frac{1}{2}$  + *y*,  $\frac{1}{2}$  - *z*]. These interactions result in the formation of interconnected 22-membered [SnCl...HCNCSnCl...HCCH...ClSnCl...HCCNCS] rings. Successive layers are separated by hydrophobic interactions.

## Experimental

The compound Cl<sub>3</sub>Sn(CMe<sub>2</sub>CH<sub>2</sub>COMe) was prepared from SnCl<sub>2</sub>, HCl and acetone according to a literature preparation (Burley *et al.*, 1984). Solutions of Cl<sub>3</sub>Sn(CMe<sub>2</sub>CH<sub>2</sub>COMe) (1.60 g), in Me<sub>2</sub>CO (20 ml), and NaS<sub>2</sub>CNEt<sub>2</sub>·3H<sub>2</sub>O (Aldrich, 1.13 g) in Me<sub>2</sub>CO (20 ml) were mixed and heated at 313 K for 30 min. The reaction mixture was cooled, filtered and the filtrate rotary evaporated to give a solid residue. The residue was recrystallized from EtOH to yield colorless crystals of (I) (m.p. 472–444 K). IR (KBr, cm<sup>-1</sup>): 1665 (ν C—O), 1440 (ν C—N), 990 (ν C—S).

### Crystal data

[SnCl<sub>2</sub>(C<sub>5</sub>H<sub>10</sub>NS<sub>2</sub>)(C<sub>6</sub>H<sub>11</sub>O)]  
*M<sub>r</sub>* = 437.00  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.487 (2) Å  
*b* = 10.870 (3) Å  
*c* = 15.319 (4) Å  
 β = 98.999 (5)°  
*V* = 1724.8 (7) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.683 Mg m<sup>-3</sup>  
 Mo Kα radiation  
 μ = 2.02 mm<sup>-1</sup>  
*T* = 150 (2) K  
 Block, colorless  
 0.45 × 0.25 × 0.25 mm

### Data collection

Rigaku AFC12K/SATURN724  
 diffractometer  
 ω scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.665, *T<sub>max</sub>* = 1  
 (expected range = 0.401–0.603)

41091 measured reflections  
 3921 independent reflections  
 3902 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.028  
 θ<sub>max</sub> = 27.5°

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.021  
*wR* (*F*<sup>2</sup>) = 0.057  
*S* = 1.20  
 3921 reflections  
 164 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2 + 1.6599P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 (Δ/σ)<sub>max</sub> = 0.001  
 Δρ<sub>max</sub> = 0.49 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.50 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Sn—Cl1	2.4509 (6)	Sn—O1	2.4026 (15)
Sn—Cl2	2.4153 (6)	S1—C1	1.743 (2)
Sn—S1	2.4720 (6)	S2—C1	1.721 (2)
Sn—S2	2.6493 (7)	O1—C8	1.226 (3)
Sn—C6	2.1832 (19)	N1—C1	1.318 (2)
Cl1—Sn—Cl2	97.09 (3)	S2—Sn—C6	101.95 (6)
Cl1—Sn—S1	87.09 (2)	S2—Sn—O1	81.74 (4)
Cl1—Sn—S2	156.763 (17)	O1—Sn—C6	76.71 (7)
Cl1—Sn—O1	90.31 (5)	Sn—S1—C1	88.80 (7)
Cl1—Sn—C6	97.35 (6)	Sn—S2—C1	83.63 (7)
Cl2—Sn—S1	98.35 (2)	Sn—O1—C8	111.12 (13)
Cl2—Sn—S2	91.99 (2)	C1—N1—C2	122.41 (17)
Cl2—Sn—O1	172.42 (4)	C1—N1—C4	122.08 (18)
Cl2—Sn—C6	100.59 (6)	C2—N1—C4	115.51 (16)
S1—Sn—S2	70.408 (19)	S2—C1—S1	117.15 (11)
S1—Sn—O1	83.63 (4)	S1—C1—N1	119.59 (15)
S1—Sn—C6	159.83 (5)	S2—C1—N1	123.26 (15)

The H atoms were included in the riding-model approximation, with methyl C—H = 0.98 Å and methylene C—H = 0.99 Å, and with *U<sub>iso</sub>*(H) = 1.2 and 1.5 *U<sub>eq</sub>*(C) for methylene and methyl H atoms, respectively.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve

structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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