Crystal structure of bis[(*O*-benzylthiocarbonato)- μ_2 -benzyloxo- μ_3 -oxo-tetramethylditin], [(benzylOCS₂)Me₂Sn(Obenzyl)OSnMe₂]₂

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Source of material: Crystals were obtained from the attempted recrystallisation of Me₂Sn(S₂CObenzyl)₂ from a dichloromethane solution of the compound; mp 401 K – 402 K.

The structure featuring a centrosymmetric R₈Sn₄O₄ ladder framework is in essential agreement with the recent report of [(iPrOC S₂)Me₂Sn(OEt)OSnMe₂]₂ (see ref. 1). Such tetrameric structures are common in analogous carboxylate chemistry where they are often formed from the decomposition/hydrolysis of R₂Sn(O₂CR')₂ (see ref. 2). In the present structure the *d*(Sn2–S1) and *d*(Sn2–S2) of 2.591(2) Å and 3.263(3) Å, respectively indicate that the xanthate coordinates in the monodentate mode and thus, that both tin centers exist in distorted trigonal bipyramidal environment.

C₁₉H₂₆O₃S₂Sn₂, triclinic, *P* $\bar{1}$ (No. 2), *a* = 10.151(8) Å, *b* = 12.603(4) Å, *c* = 9.618(5) Å, α = 96.67(3)°, β = 97.67(5)°, γ = 82.58(4)°, *V* = 1203.1 Å³, *Z* = 2, *R*(*F*) = 0.046, *R*_w(*F*) = 0.055.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless block, size 0.10 x 0.16 x 0.47 mm
Wavelength:	Mo K α radiation (0.7107 Å)
μ :	22.63 cm ⁻¹
Diffractometer:	AFC6R
Scan mode:	$\omega/2\theta$
<i>T</i> _{measurement} :	293 K
$2\theta_{\text{max}}$:	55.2°
<i>N</i> (<i>hkl</i>) _{unique} :	3848
Criterion for <i>F</i> _o :	<i>F</i> _o > 6 σ (<i>F</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	236
Program:	TEXSAN

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	2i	0.6958	0.7914	0.2794	0.1040
H(2)	2i	0.6185	0.8316	0.4118	0.1040
H(3)	2i	0.6248	0.9318	0.0811	0.1164
H(4)	2i	0.6407	1.1107	0.0537	0.1557
H(5)	2i	0.6667	1.2338	0.2507	0.1583
H(6)	2i	0.6563	1.1807	0.4732	0.1541
H(7)	2i	0.6432	1.0041	0.4988	0.1135
H(8)	2i	0.1215	0.3394	0.4179	0.3057
H(9)	2i	0.2737	0.3049	0.3964	0.3057
H(10)	2i	0.3234	0.1520	0.2357	0.1819
H(11)	2i	0.2847	-0.0310	0.1729	0.2378
H(12)	2i	0.0809	-0.0720	0.2216	0.2593
H(13)	2i	-0.0570	0.0226	0.3429	0.3235
H(14)	2i	-0.0151	0.2057	0.4049	0.2532
H(15)	2i	0.1503	0.2606	-0.0857	0.1249
H(16)	2i	0.0693	0.1891	-0.0107	0.1249
H(17)	2i	-0.0016	0.2488	-0.1416	0.1249
H(18)	2i	-0.1407	0.4766	0.2748	0.1107
H(19)	2i	-0.1500	0.3512	0.2586	0.1107
H(20)	2i	-0.2375	0.4247	0.1497	0.1107
H(21)	2i	0.3880	0.3713	0.0478	0.1345
H(22)	2i	0.4926	0.4521	0.1132	0.1345
H(23)	2i	0.4663	0.3591	0.2000	0.1345
H(24)	2i	0.2599	0.5241	0.4937	0.1270
H(25)	2i	0.2581	0.6428	0.4538	0.1270
H(26)	2i	0.1257	0.5856	0.4240	0.1270

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Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Sn(1)	2i	0.00398(5)	0.38894(3)	0.07894(5)	0.0549(3)	0.0504(3)	0.0552(3)	−0.0086(2)	0.0066(2)	0.0132(2)
Sn(2)	2i	0.27261(5)	0.51291(3)	0.22369(5)	0.0529(3)	0.0509(3)	0.0577(3)	−0.0036(2)	0.0012(2)	0.0072(2)
S(1)	2i	0.5404(3)	0.6266(2)	0.3505(3)	0.106(2)	0.071(1)	0.147(2)	−0.023(1)	−0.056(2)	0.038(1)
S(2)	2i	0.3101(2)	0.6937(2)	0.1402(2)	0.062(1)	0.065(1)	0.080(1)	−0.0159(9)	−0.0059(9)	0.0211(9)
O(1)	2i	0.1061(4)	0.5181(3)	0.0823(4)	0.046(2)	0.054(2)	0.057(3)	−0.007(2)	0.002(2)	0.014(2)
O(2)	2i	0.1678(5)	0.3684(4)	0.2403(5)	0.090(4)	0.065(3)	0.078(3)	−0.023(3)	−0.021(3)	0.037(3)
O(3)	2i	0.4956(5)	0.8082(4)	0.2316(5)	0.061(3)	0.062(3)	0.094(4)	−0.016(2)	−0.010(3)	0.017(3)
C(1)	2i	0.4565(7)	0.7133(5)	0.2456(7)	0.064(5)	0.057(4)	0.073(4)	−0.006(4)	0.004(4)	0.004(3)
C(2)	2i	0.6202(8)	0.8380(7)	0.313(1)	0.071(5)	0.078(5)	0.111(6)	−0.023(4)	−0.015(5)	0.025(5)
C(3)	2i	0.6310(7)	0.9520(6)	0.2911(9)	0.047(4)	0.070(5)	0.093(6)	−0.016(4)	0.004(4)	0.014(4)
C(4)	2i	0.632(1)	0.9831(8)	0.162(1)	0.104(8)	0.102(7)	0.089(6)	−0.015(6)	0.007(6)	0.024(5)
C(5)	2i	0.642(1)	1.089(1)	0.145(2)	0.091(8)	0.15(1)	0.16(1)	−0.022(9)	0.002(8)	0.079(9)
C(6)	2i	0.655(1)	1.1615(9)	0.261(2)	0.074(7)	0.087(8)	0.25(2)	−0.009(6)	0.01(1)	0.08(1)
C(7)	2i	0.652(1)	1.1295(9)	0.393(2)	0.102(8)	0.074(7)	0.21(1)	−0.026(6)	0.050(9)	−0.036(8)
C(8)	2i	0.6422(9)	1.0261(8)	0.407(1)	0.091(7)	0.094(7)	0.106(7)	−0.034(6)	0.023(5)	0.004(5)
C(9)	2i	0.182(2)	0.305(1)	0.352(2)	0.38(2)	0.15(1)	0.23(1)	−0.15(1)	−0.21(2)	0.14(1)
C(10)	2i	0.156(1)	0.1947(6)	0.322(1)	0.078(6)	0.052(4)	0.110(7)	−0.012(4)	−0.033(5)	0.034(4)
C(11)	2i	0.244(1)	0.127(1)	0.257(1)	0.17(1)	0.15(1)	0.14(1)	0.05(1)	0.06(1)	0.08(1)
C(12)	2i	0.224(2)	0.021(1)	0.218(2)	0.31(3)	0.11(1)	0.14(1)	0.08(1)	−0.01(1)	0.00(1)
C(13)	2i	0.102(2)	−0.001(2)	0.255(3)	0.19(2)	0.16(2)	0.31(3)	−0.13(2)	−0.08(2)	0.09(2)
C(14)	2i	0.018(2)	0.050(2)	0.318(4)	0.08(1)	0.14(2)	0.59(5)	0.01(1)	0.00(2)	0.11(2)
C(15)	2i	0.046(1)	0.157(1)	0.352(2)	0.10(1)	0.10(1)	0.41(3)	0.047(8)	0.03(1)	0.05(1)
C(16)	2i	0.064(1)	0.2536(7)	−0.058(1)	0.099(7)	0.070(5)	0.120(7)	0.014(5)	−0.022(6)	−0.022(5)
C(17)	2i	−0.1521(9)	0.4137(8)	0.2079(9)	0.081(6)	0.131(8)	0.076(5)	−0.034(6)	0.031(5)	0.009(5)
C(18)	2i	0.4254(9)	0.4100(7)	0.134(1)	0.068(6)	0.090(6)	0.17(1)	0.009(5)	0.026(6)	−0.023(6)
C(19)	2i	0.222(1)	0.5747(7)	0.4262(9)	0.16(1)	0.095(7)	0.062(5)	−0.014(6)	0.031(6)	−0.004(4)

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References

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