Crystal structure of 2,2,4,4-tetrakis-(tri-*tert*-butoxysilanethiolato)-1,3,2,4-dithiadistannetane, $[\text{Si}(\text{OC}_4\text{H}_9)_3]_4\text{Sn}_2\text{S}_6$

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Source of material: The title compound was obtained from (*tert*-C₄H₉O)₃SiSH (see ref. 1), sulfur, and (C₂H₅)₃N with SnCl₂ in toluene solution at 343 K; recrystallization from benzene.

The positions of all terminal C atoms were refined isotropically, due to their high thermal motion. The positions of the H atoms were calculated by riding model and considered with $U_{\text{iso}} = 1.2 \times U_{\text{iso}}$ of the corresponding C atom.

C₄₈H₁₀₈O₁₂S₆Si₄Sn₂, orthorhombic, *Pbca* (No. 61), $a = 19.037(3) \text{ \AA}$, $b = 12.761(2) \text{ \AA}$, $c = 30.510(5) \text{ \AA}$, $V = 7412.1 \text{ \AA}^3$, $Z = 4$, $R(F) = 0.066$, $R_w(F) = 0.067$.

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

Crystal:	colorless plate, size 0.75 x 0.8 x 0.52 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	9.40 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	8518
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	236
Program:	SHELXTL-plus

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

Atom	Site	x	y	z	U_{iso}
C(11)	8c	0.1001(6)	0.9356(9)	0.4188(4)	0.129(4)
H(11A)	8c	0.1219(6)	0.9319(9)	0.4471(4)	0.16
H(11B)	8c	0.0815(6)	1.0047(9)	0.4143(4)	0.16
H(11C)	8c	0.1342(6)	0.9203(9)	0.3965(4)	0.16
C(12)	8c	-0.0145(5)	0.8716(8)	0.4505(3)	0.109(4)
H(12A)	8c	-0.0332(5)	0.9414(8)	0.4490(3)	0.13
H(12B)	8c	0.0054(5)	0.8602(8)	0.4790(3)	0.13
H(12C)	8c	-0.0515(5)	0.8219(8)	0.4455(3)	0.13
C(13)	8c	0.0085(5)	0.8653(8)	0.3711(3)	0.107(4)
H(13A)	8c	-0.0092(5)	0.9348(8)	0.3664(3)	0.13
H(13B)	8c	-0.0295(5)	0.8161(8)	0.3696(3)	0.13
H(13C)	8c	0.0426(5)	0.8490(8)	0.3490(3)	0.13
C(21)	8c	0.1926(9)	0.735(1)	0.5086(6)	0.240(9)
H(21A)	8c	0.1536(9)	0.687(1)	0.5084(6)	0.33
H(21B)	8c	0.1758(9)	0.805(1)	0.5042(6)	0.33
H(21C)	8c	0.2163(9)	0.731(1)	0.5363(6)	0.33
C(22)	8c	0.2914(9)	0.794(1)	0.4816(6)	0.246(9)
H(22A)	8c	0.3272(9)	0.784(1)	0.4599(6)	0.31
H(22B)	8c	0.3117(9)	0.788(1)	0.5103(6)	0.31
H(22C)	8c	0.2711(9)	0.863(1)	0.4782(6)	0.31
C(23)	8c	0.277(1)	0.613(1)	0.4806(6)	0.27(1)
H(23A)	8c	0.243(1)	0.557(1)	0.4773(6)	0.37
H(23B)	8c	0.297(1)	0.610(1)	0.5094(6)	0.37
H(23C)	8c	0.313(1)	0.605(1)	0.4590(6)	0.37
C(31)	8c	0.1893(6)	0.7023(9)	0.2823(4)	0.135(4)
H(31A)	8c	0.2289(6)	0.6974(9)	0.2629(4)	0.16
H(31B)	8c	0.1606(6)	0.7609(9)	0.2739(4)	0.16
H(31C)	8c	0.1622(6)	0.6391(9)	0.2805(4)	0.16
C(32)	8c	0.2623(6)	0.6240(9)	0.3398(4)	0.133(4)
H(32A)	8c	0.2788(6)	0.6330(9)	0.3693(4)	0.16
H(32B)	8c	0.3017(6)	0.6223(9)	0.3201(4)	0.16
H(32C)	8c	0.2368(6)	0.5593(9)	0.3376(4)	0.16
C(33)	8c	0.2556(6)	0.8169(9)	0.3319(4)	0.126(4)
H(33A)	8c	0.2962(6)	0.8146(9)	0.3134(4)	0.15
H(33B)	8c	0.2701(6)	0.8265(9)	0.3618(4)	0.15
H(33C)	8c	0.2260(6)	0.8741(9)	0.3233(4)	0.15
C(41)	8c	-0.2588(9)	0.397(1)	0.3091(5)	0.199(7)
H(41A)	8c	-0.2505(9)	0.323(1)	0.3067(5)	0.28
H(41B)	8c	-0.2267(9)	0.434(1)	0.2904(5)	0.28
H(41C)	8c	-0.3062(9)	0.412(1)	0.3005(5)	0.28
C(42)	8c	-0.2981(9)	0.376(1)	0.3802(6)	0.231(9)
H(42A)	8c	-0.2926(9)	0.395(1)	0.4103(6)	0.28
H(42B)	8c	-0.2905(9)	0.302(1)	0.3771(6)	0.28
H(42C)	8c	-0.3447(9)	0.393(1)	0.3706(6)	0.28
C(43)	8c	-0.2627(9)	0.542(1)	0.3524(5)	0.206(8)
H(43A)	8c	-0.2571(9)	0.572(1)	0.3809(5)	0.25
H(43B)	8c	-0.3099(9)	0.552(1)	0.3424(5)	0.25
H(43C)	8c	-0.2305(9)	0.574(1)	0.3323(5)	0.25
C(51)	8c	-0.0732(5)	0.1954(7)	0.3974(3)	0.095(3)
H(51A)	8c	-0.0660(5)	0.1233(7)	0.3898(3)	0.11

Table 2. (Continued)

Atom	Site	x	y	z	U _{iso}
H(51B)	8c	-0.1226(5)	0.2107(7)	0.3970(3)	0.11
H(51C)	8c	-0.0548(5)	0.2083(7)	0.4262(3)	0.11
C(52)	8c	0.0435(5)	0.2510(8)	0.3673(4)	0.117(4)
H(52A)	8c	0.0551(5)	0.1799(8)	0.3600(4)	0.14
H(52B)	8c	0.0587(5)	0.2656(8)	0.3967(4)	0.14
H(52C)	8c	0.0666(5)	0.2977(8)	0.3473(4)	0.14
C(53)	8c	-0.0611(5)	0.2409(8)	0.3193(3)	0.097(3)
H(53A)	8c	-0.0527(5)	0.1683(8)	0.3129(3)	0.11
H(53B)	8c	-0.0367(5)	0.2837(8)	0.2984(3)	0.11
H(53C)	8c	-0.1106(5)	0.2549(8)	0.3176(3)	0.11
C(61)	8c	-0.0695(6)	0.5079(8)	0.2383(4)	0.126(4)

Table 2. (Continued)

Atom	Site	x	y	z	U _{iso}
H(61A)	8c	-0.0414(6)	0.5432(8)	0.2168(4)	0.15
H(61B)	8c	-0.1183(6)	0.5166(8)	0.2313(4)	0.15
H(61C)	8c	-0.0580(6)	0.4347(8)	0.2385(4)	0.15
C(62)	8c	0.0153(8)	0.550(1)	0.2925(5)	0.208(8)
H(62A)	8c	0.0226(8)	0.580(1)	0.3210(5)	0.27
H(62B)	8c	0.0398(8)	0.591(1)	0.2710(5)	0.27
H(62C)	8c	0.0327(8)	0.479(1)	0.2920(5)	0.27
C(63)	8c	-0.0858(8)	0.665(1)	0.2836(5)	0.202(7)
H(63A)	8c	-0.0586(8)	0.710(1)	0.2648(5)	0.25
H(63B)	8c	-0.0838(8)	0.691(1)	0.3131(5)	0.25
H(63C)	8c	-0.1337(8)	0.665(1)	0.2738(5)	0.25

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)	8c	0.00678(2)	0.53252(4)	0.44822(1)	0.0523(3)	0.0494(3)	0.0427(2)	-0.0034(2)	0.0011(2)	0.0016(2)
S(1)	8c	0.1165(1)	0.5310(1)	0.41077(7)	0.061(1)	0.051(1)	0.079(1)	0.0014(9)	0.0174(9)	0.001(1)
S(2)	8c	-0.0915(1)	0.5858(2)	0.40518(6)	0.069(1)	0.061(1)	0.064(1)	0.011(1)	-0.0153(9)	-0.0108(9)
S(3)	8c	-0.0032(1)	0.3667(1)	0.48546(6)	0.083(1)	0.0469(9)	0.0478(9)	-0.0089(9)	0.0008(9)	-0.0022(7)
Si(1)	8c	0.1394(1)	0.6939(2)	0.40625(7)	0.050(1)	0.054(1)	0.056(1)	-0.0036(9)	0.0044(8)	0.0078(9)
Si(2)	8c	-0.1041(1)	0.4571(2)	0.36112(6)	0.051(1)	0.060(1)	0.050(1)	-0.0023(9)	-0.0044(8)	-0.0022(9)
O(1)	8c	0.0679(3)	0.7501(4)	0.4212(2)	0.063(3)	0.055(3)	0.075(3)	0.010(2)	0.008(3)	0.009(3)
O(2)	8c	0.2070(3)	0.7264(4)	0.4334(2)	0.068(3)	0.082(4)	0.073(3)	-0.010(3)	-0.008(3)	0.011(3)
O(3)	8c	0.1546(3)	0.7240(4)	0.3559(2)	0.069(3)	0.082(4)	0.064(3)	-0.002(3)	0.010(3)	0.016(3)
O(4)	8c	-0.1802(3)	0.4050(4)	0.3680(2)	0.058(3)	0.079(4)	0.087(4)	-0.001(3)	-0.012(3)	-0.005(3)
O(5)	8c	-0.0466(3)	0.3738(4)	0.3762(2)	0.074(4)	0.067(3)	0.066(3)	0.015(3)	-0.012(3)	-0.014(3)
O(6)	8c	-0.1018(3)	0.4930(5)	0.3116(2)	0.098(4)	0.097(4)	0.052(3)	-0.016(4)	-0.002(3)	0.003(3)
C(1)	8c	0.0422(4)	0.8590(6)	0.4159(3)	0.067(5)	0.052(4)	0.085(6)	0.008(4)	-0.000(4)	0.012(4)
C(2)	8c	0.2404(5)	0.7141(8)	0.4759(3)	0.079(6)	0.094(7)	0.080(6)	-0.005(5)	-0.017(5)	-0.000(5)
C(3)	8c	0.2152(4)	0.7159(7)	0.3274(3)	0.068(5)	0.094(6)	0.072(5)	-0.012(5)	0.015(4)	0.012(5)
C(4)	8c	-0.2494(4)	0.4307(8)	0.3543(3)	0.046(4)	0.106(7)	0.100(7)	-0.002(5)	-0.004(4)	-0.006(6)
C(5)	8c	-0.0353(4)	0.2652(6)	0.3645(3)	0.069(5)	0.072(5)	0.076(5)	0.011(4)	-0.005(4)	-0.023(4)
C(6)	8c	-0.0563(6)	0.5539(9)	0.2823(3)	0.112(8)	0.121(8)	0.056(5)	-0.034(7)	0.004(5)	0.013(5)

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