Crystal structure of tetrakis(2,2-dimethyl-2-phenylethyl)tin, C₄₀H₅₂Sn

H. Reuter and R. Pawlak

Universität Osnabrück, Institut für Chemie, Barbarastr. 7, D-49069 Osnabrück, Germany

Received February 14, 1997, CSD-No. 402850

Source of material: The title compound was obtained by reaction of neophylmagnesiumchloride in ether with tin tetrachloride in toluene (see ref. 6) and recrystallization from methanol. An empirical absorption correction was carried out using ψ -scans. The asymmetric unit contains one tetraeneophyltin molecule. Sn is tetrahedrally coordinated with C–Sn–C angles from 104.6° to 111.1°, the mean Sn–C distance is 2.186 Å. These values correspond well with those found in tetrabenzyltin (see ref. 1), tetrakis(2,2-dimethyl-1-phenylethenyl)tin (see ref. 2), tetrakis(indenyl)tin (see ref. 3), tetrakis(2-methoxybenzyl)tin (see ref. 4) and tetracyclopentadienyltin (see ref. 5).

C₄₀H₅₂Sn, monoclinic, *P*12₁/c1 (No. 14), *a* = 13.987(3) Å, *b* = 10.075(4) Å, *c* = 25.993(8) Å, β = 104.38(1)°, *V* = 3548.1 Å³, *Z* = 4, *R*(*F*) = 0.046, *R*_w(*F*²) = 0.087.

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

Crystal:	colorless, transparent block, size 0.3 x 0.3 x 0.5 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	7.44 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	2 θ / ω
<i>T</i> _{measurement} :	293 K
2 θ _{max} :	44°
<i>N</i> (<i>hkl</i>) _{unique} :	4320
Criterion for <i>I</i> _o :	<i>I</i> _o > 2 σ (<i>I</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	372
Programs:	SHELXTL, SHELXS-86, SHELXL-93

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(10A)	4e	0.5713(5)	0.4238(7)	0.1217(3)	0.079(4)
H(10B)	4e	0.5383(5)	0.3262(7)	0.0742(3)	0.079(4)
H(12A)	4e	0.3823(5)	0.289(1)	0.0952(3)	0.079(4)
H(12B)	4e	0.4123(5)	0.389(1)	0.1429(3)	0.079(4)
H(12C)	4e	0.3774(5)	0.245(1)	0.1523(3)	0.079(4)
H(13A)	4e	0.4899(7)	0.0989(9)	0.0876(4)	0.079(4)
H(13B)	4e	0.4837(7)	0.0501(9)	0.1440(4)	0.079(4)
H(13C)	4e	0.5869(7)	0.0706(9)	0.1316(4)	0.079(4)
H(15)	4e	0.5756(6)	0.4601(9)	0.2056(3)	0.079(4)
H(16)	4e	0.6542(7)	0.483(1)	0.2933(4)	0.079(4)
H(17)	4e	0.6962(7)	0.299(1)	0.3468(3)	0.079(4)
H(18)	4e	0.6588(8)	0.093(1)	0.3108(4)	0.079(4)
H(19)	4e	0.5751(6)	0.0669(9)	0.2230(4)	0.079(4)
H(20A)	4e	0.8075(5)	0.0950(7)	0.0705(3)	0.079(4)
H(20B)	4e	0.6988(5)	0.0567(7)	0.0685(3)	0.079(4)
H(22A)	4e	0.5637(5)	0.125(1)	-0.0073(3)	0.079(4)
H(22B)	4e	0.5874(5)	0.190(1)	-0.0577(3)	0.079(4)
H(22C)	4e	0.5978(5)	0.274(1)	-0.0059(3)	0.079(4)
H(23A)	4e	0.6799(7)	-0.0570(9)	-0.0147(3)	0.079(4)
H(23B)	4e	0.7904(7)	-0.0250(9)	-0.0129(3)	0.079(4)
H(23C)	4e	0.7069(7)	0.0128(9)	-0.0631(3)	0.079(4)
H(25)	4e	0.9086(6)	0.148(1)	0.0222(4)	0.079(4)
H(26)	4e	1.0170(8)	0.287(2)	-0.0032(4)	0.079(4)
H(27)	4e	0.9629(9)	0.453(2)	-0.0639(5)	0.079(4)
H(28)	4e	0.7980(9)	0.490(1)	-0.0936(4)	0.079(4)
H(29)	4e	0.6853(7)	0.3574(9)	-0.0665(3)	0.079(4)
H(30A)	4e	0.8602(6)	0.4836(8)	0.1119(3)	0.079(4)
H(30B)	4e	0.8102(6)	0.4502(8)	0.0528(3)	0.079(4)
H(32A)	4e	0.8717(7)	0.717(1)	0.1009(4)	0.079(4)
H(32B)	4e	0.7836(7)	0.797(1)	0.0654(4)	0.079(4)
H(32C)	4e	0.8380(7)	0.689(1)	0.0397(4)	0.079(4)
H(33A)	4e	0.6101(7)	0.535(1)	0.0378(3)	0.079(4)
H(33B)	4e	0.6788(7)	0.578(1)	0.0014(3)	0.079(4)
H(33C)	4e	0.6244(7)	0.686(1)	0.0270(3)	0.079(4)
H(35)	4e	0.5799(6)	0.724(1)	0.0981(4)	0.079(4)
H(36)	4e	0.5467(9)	0.7968(9)	0.1774(6)	0.079(4)
H(37)	4e	0.658(1)	0.758(1)	0.2563(5)	0.079(4)
H(38)	4e	0.8044(9)	0.660(1)	0.2586(4)	0.079(4)
H(39)	4e	0.8369(7)	0.5851(9)	0.1826(3)	0.079(4)
H(40A)	4e	0.8572(5)	0.3354(7)	0.2046(3)	0.079(4)
H(40B)	4e	0.7717(5)	0.2495(7)	0.2154(3)	0.079(4)
H(42A)	4e	0.8933(6)	0.145(1)	0.2856(3)	0.079(4)
H(42B)	4e	0.9798(6)	0.223(1)	0.2713(3)	0.079(4)
H(42C)	4e	0.9831(6)	0.068(1)	0.2739(3)	0.079(4)
H(43A)	4e	0.7793(7)	0.0107(9)	0.2177(5)	0.079(4)
H(43B)	4e	0.8714(7)	-0.0657(9)	0.2086(5)	0.079(4)
H(43C)	4e	0.7951(7)	-0.0025(9)	0.1603(5)	0.079(4)
H(45)	4e	0.9665(8)	-0.058(1)	0.1542(5)	0.079(4)
H(46)	4e	1.087(1)	-0.046(2)	0.1099(6)	0.079(4)
H(47)	4e	1.160(1)	0.149(2)	0.0998(5)	0.079(4)
H(48)	4e	1.1132(8)	0.339(2)	0.1350(5)	0.079(4)
H(49)	4e	0.9895(6)	0.334(1)	0.1775(4)	0.079(4)

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)	4e	0.72989(4)	0.29503(5)	0.11213(2)	0.0402(2)	0.0389(3)	0.0403(3)	−0.0001(3)	0.0114(2)	0.0006(3)
C(10)	4e	0.5757(5)	0.3323(7)	0.1109(3)	0.049(4)	0.049(5)	0.036(4)	−0.001(4)	0.013(3)	0.006(3)
C(11)	4e	0.5219(5)	0.2473(7)	0.1437(3)	0.039(4)	0.056(5)	0.060(5)	−0.007(3)	0.018(4)	−0.003(4)
C(12)	4e	0.4130(5)	0.297(1)	0.1325(3)	0.049(4)	0.105(7)	0.065(5)	0.007(6)	0.020(4)	0.001(7)
C(13)	4e	0.5205(7)	0.1033(9)	0.1250(4)	0.079(6)	0.074(6)	0.076(6)	−0.027(5)	0.027(5)	−0.012(5)
C(14)	4e	0.5696(5)	0.2608(8)	0.2028(3)	0.044(4)	0.052(5)	0.058(5)	−0.008(3)	0.022(4)	0.008(4)
C(15)	4e	0.5925(6)	0.3843(9)	0.2263(3)	0.075(6)	0.054(5)	0.059(6)	−0.004(5)	0.028(5)	0.001(5)
C(16)	4e	0.6393(7)	0.398(1)	0.2791(4)	0.092(7)	0.082(7)	0.058(6)	−0.018(6)	0.029(5)	−0.019(6)
C(17)	4e	0.6643(7)	0.289(1)	0.3111(3)	0.097(7)	0.107(8)	0.042(5)	−0.016(8)	0.012(5)	0.004(7)
C(18)	4e	0.6415(8)	0.167(1)	0.2895(4)	0.083(7)	0.10(1)	0.067(7)	−0.003(6)	0.022(6)	0.036(6)
C(19)	4e	0.5926(6)	0.1516(9)	0.2363(4)	0.065(5)	0.059(6)	0.075(7)	−0.013(5)	0.021(5)	0.009(5)
C(20)	4e	0.7400(5)	0.1269(7)	0.0602(3)	0.050(4)	0.040(4)	0.049(5)	−0.002(4)	0.011(3)	−0.004(4)
C(21)	4e	0.7127(6)	0.1432(8)	−0.0003(3)	0.057(5)	0.056(5)	0.043(4)	−0.002(4)	0.007(4)	−0.008(4)
C(22)	4e	0.6055(5)	0.187(1)	−0.0196(3)	0.055(4)	0.077(6)	0.059(5)	0.007(5)	0.007(4)	−0.004(5)
C(23)	4e	0.7235(7)	0.0053(9)	−0.0251(3)	0.081(6)	0.064(6)	0.059(5)	−0.014(5)	0.019(5)	−0.021(5)
C(24)	4e	0.7831(5)	0.2363(8)	−0.0182(3)	0.057(5)	0.057(5)	0.032(4)	−0.005(4)	0.013(3)	−0.011(4)
C(25)	4e	0.8845(6)	0.218(1)	−0.0008(4)	0.064(5)	0.088(7)	0.073(6)	0.005(6)	0.023(5)	0.006(6)
C(26)	4e	0.9496(8)	0.300(2)	−0.0168(4)	0.071(6)	0.14(1)	0.092(7)	−0.023(9)	0.031(6)	0.002(9)
C(27)	4e	0.9179(9)	0.400(2)	−0.0523(5)	0.097(9)	0.14(1)	0.086(8)	−0.050(9)	0.034(7)	−0.001(8)
C(28)	4e	0.8205(9)	0.421(1)	−0.0700(4)	0.12(1)	0.087(8)	0.065(6)	−0.021(7)	0.030(6)	0.023(6)
C(29)	4e	0.7524(7)	0.3409(9)	−0.0536(3)	0.080(6)	0.078(7)	0.042(5)	−0.008(5)	0.014(4)	−0.002(5)
C(30)	4e	0.7968(6)	0.4711(8)	0.0868(3)	0.059(5)	0.047(5)	0.060(5)	0.001(4)	0.028(4)	0.003(4)
C(31)	4e	0.7435(5)	0.6065(8)	0.0805(3)	0.052(4)	0.041(5)	0.056(5)	0.005(4)	0.016(4)	0.008(4)
C(32)	4e	0.8160(7)	0.712(1)	0.0707(4)	0.107(7)	0.049(5)	0.097(7)	0.008(6)	0.056(6)	0.023(6)
C(33)	4e	0.6562(7)	0.601(1)	0.0322(3)	0.097(7)	0.071(6)	0.052(5)	0.001(6)	0.014(5)	0.009(5)
C(34)	4e	0.7141(5)	0.6482(7)	0.1321(3)	0.052(5)	0.031(4)	0.058(5)	0.000(3)	0.020(4)	0.003(3)
C(35)	4e	0.6257(6)	0.710(1)	0.1303(4)	0.064(5)	0.065(5)	0.090(6)	0.014(6)	0.021(5)	0.004(6)
C(36)	4e	0.6057(9)	0.7533(9)	0.1780(6)	0.114(9)	0.054(6)	0.16(1)	0.019(6)	0.095(9)	−0.010(7)
C(37)	4e	0.672(1)	0.732(1)	0.2248(5)	0.18(1)	0.071(8)	0.089(8)	−0.042(9)	0.081(9)	−0.028(7)
C(38)	4e	0.7583(9)	0.672(1)	0.2264(4)	0.114(8)	0.081(8)	0.066(6)	−0.026(7)	0.024(6)	−0.016(6)
C(39)	4e	0.7777(7)	0.6292(9)	0.1808(3)	0.068(5)	0.058(5)	0.057(5)	−0.014(5)	0.011(5)	−0.009(5)
C(40)	4e	0.8175(5)	0.2569(7)	0.1930(3)	0.049(4)	0.049(5)	0.048(4)	−0.001(3)	0.002(3)	0.007(3)
C(41)	4e	0.8868(5)	0.1369(8)	0.2050(3)	0.044(4)	0.049(4)	0.065(5)	−0.002(4)	0.007(4)	0.009(4)
C(42)	4e	0.9409(6)	0.144(1)	0.2646(3)	0.057(5)	0.087(7)	0.075(6)	0.002(5)	0.005(4)	0.013(5)
C(43)	4e	0.8277(7)	0.0079(9)	0.1972(5)	0.079(7)	0.054(6)	0.120(9)	−0.011(5)	0.005(6)	0.020(6)
C(44)	4e	0.9637(5)	0.1358(9)	0.1732(3)	0.042(4)	0.057(5)	0.060(5)	0.012(4)	0.005(4)	0.012(4)
C(45)	4e	0.9953(8)	0.024(1)	0.1509(5)	0.077(7)	0.081(8)	0.14(1)	0.012(6)	0.023(7)	−0.032(7)
C(46)	4e	1.067(1)	0.031(2)	0.1242(6)	0.10(1)	0.16(2)	0.14(1)	0.04(1)	0.045(9)	−0.06(1)
C(47)	4e	1.110(1)	0.146(2)	0.1181(5)	0.079(9)	0.27(3)	0.074(8)	0.03(1)	0.029(7)	0.02(1)
C(48)	4e	1.0824(8)	0.259(2)	0.1388(5)	0.072(7)	0.16(2)	0.110(9)	0.012(8)	0.036(7)	0.05(1)
C(49)	4e	1.0097(6)	0.256(1)	0.1648(4)	0.064(5)	0.076(7)	0.097(7)	0.012(5)	0.034(5)	0.032(5)

References

1. Davies, G. R.; Jarvis, J. A. J.; Kilbourn, T.: Crystal and molecular structures (at −40°C) of the tetrabenzyls of titanium, hafnium, and tin. *J. Chem. Soc. D* (1971) 1511.
2. Cardin, C. J.; Cardin, D. J.; Kelly, J. M.; Norton, R. J.; Roy, A.; Hathaway, B. J.; King, T. J.: Synthesis, Properties, and X-Ray Crystal and Molecular Structures of Homoleptic Alkenyls of Tin and Chromium. *J. Chem. Soc. Dalton Trans.* (1983) 671.
3. Atwood, J. L.; McMaster, A. D.; Rogers, R. D.; Stobart, S. R.: Stereochemically Nonrigid Silanes, Germanes, and Stannanes. 12. Crystal and Molecular Structures of Tetrakis(indenyl) Derivatives of Germanium and Tin: Meso Diastereomers with S₄ Symmetry. *Organometallics* 3 (1984) 1500.
4. Ross, J.; Wardell, J. L.; Ferguson, G.; Low, J. N.: Symmetrical Tetrasubstituted Tin Compounds: Tetrakis(2-methoxyphenyl)tin and Tetrakis(2-methoxybenzyl)tin. *Acta Crystallogr. C* 50 (1994) 1703.
5. Kulishov, V. I.; Bokii, N. G.; Prikhotko, A. F.; Struchkov, Y. T.: Crystal structure of polycyclopentadienyl compounds of metals. III. Structure of tetracyclopentadienyltin at −60°C. *Zh. Strukt. Khim.* 16 (1975) 252.
6. Reichle, W. T.: Tetraneophyltin and Its Derivatives: The Effects of Steric Hindrance in Organotin Chemistry. *Inorg. Chem.* 5 (1966) 87-91.
7. Sheldrick, G. M.: Program Package SHELXTL. Release 5, Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1994.
8. Sheldrick, G. M.: SHELXS-86, Program for crystal structure refinement. University of Göttingen, Germany 1986.
9. Sheldrick, G. M.: SHELXL-93, Program for crystal structure refinement. University of Göttingen, Germany 1993.