Crystal structure of *catena*-poly-(μ -acetato)triphenyltin—chloroform (2/1), $\text{Ph}_3\text{Sn}(\text{O}_2\text{CMe}) \cdot 0.5\text{CHCl}_3$

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Abstract

$\text{C}_{41}\text{H}_{37}\text{Cl}_3\text{O}_4\text{Sn}_2$, monoclinic, $P12_1/n1$ (No. 14), $a = 10.213(4)$ Å, $b = 17.005(5)$ Å, $c = 23.524(4)$ Å, $\beta = 92.34(2)^\circ$, $V = 4082.1$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.051$, $wR(F) = 0.051$, $T = 293$ K.

Source of material

The preparation of the compound was as per the literature method [1]. Crystals were obtained by layering a solution of petroleum spirit (373 K–393 K) into a chloroform solution of the compound.

Discussion

The asymmetric unit comprises two $\text{Ph}_3\text{Sn}(\text{O}_2\text{CMe})$ entities and one molecule of CHCl_3 . Each tin atom exists in a distorted trigonal bipyramidal environment in which the trigonal plane is defined by the three ipso C atoms of the phenyl groups. The axial positions are occupied by two oxygen atoms, one of which is derived from a symmetry related carboxylate ligand. The overall structure is therefore polymeric as a result of the bidentate bridging carboxylate ligands. The structure reported here resembles closely that found for the unsolvated compound [1]. Both forms of the structure conform to the predominant motif found for $\text{R}_3\text{Sn}(\text{O}_2\text{CR}')$ structures [2–4]. Small differences in tin–ligand parameters found between the unsolvated and solvated forms of $[\text{Ph}_3\text{Sn}(\text{O}_2\text{CMe})]_n$ may be ascribed to the influence of crystal packing effects [5].

Table 1. Data collection and handling.

Crystal:	colourless block, size $0.13 \times 0.18 \times 0.40$ mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ :	14.57 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC6R, $\omega/2\theta$
$2\theta_{\text{max}}$:	55.2°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	10288, 9761
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 3 \sigma(I_{\text{obs}})$, 3841
$N(\text{param})_{\text{refined}}$:	451
Programs:	teXsan [6], DIRDIF [7], DIFABS [8]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(2a)	4e	0.2309	0.4407	0.0548	0.090
H(2b)	4e	0.2188	0.3641	0.0166	0.090
H(2c)	4e	0.0911	0.4106	0.0327	0.090
H(4a)	4e	−0.1895	0.1739	0.3074	0.100
H(4b)	4e	−0.1698	0.1826	0.2412	0.100
H(4c)	4e	−0.2355	0.1057	0.2652	0.100
H(12)	4e	0.3213	0.2047	0.2525	0.083
H(13)	4e	0.5417	0.1669	0.2501	0.111
H(14)	4e	0.6193	0.1048	0.1696	0.108
H(15)	4e	0.4797	0.0876	0.0888	0.102
H(16)	4e	0.2552	0.1268	0.0921	0.080
H(22)	4e	0.0946	0.3028	0.2874	0.090
H(23)	4e	−0.0114	0.4124	0.3276	0.111
H(24)	4e	−0.1934	0.4668	0.2821	0.114
H(25)	4e	−0.2567	0.4259	0.1914	0.106
H(26)	4e	−0.1460	0.3259	0.1479	0.087
H(32)	4e	−0.0613	0.0408	0.1674	0.087
H(33)	4e	−0.1956	−0.0366	0.1066	0.111
H(34)	4e	−0.2785	0.0150	0.0201	0.116
H(35)	4e	−0.2213	0.1433	−0.0067	0.095
H(36)	4e	−0.0771	0.2183	0.0523	0.082
H(42)	4e	0.3339	0.6363	0.1147	0.093
H(43)	4e	0.1592	0.7214	0.0827	0.137
H(44)	4e	−0.0550	0.6835	0.0943	0.131
H(45)	4e	−0.1026	0.5662	0.1369	0.126
H(46)	4e	0.0635	0.4814	0.1668	0.092
H(52)	4e	0.5671	0.5192	0.0762	0.085
H(53)	4e	0.7121	0.4594	0.0129	0.108
H(54)	4e	0.7370	0.3218	0.0154	0.096
H(55)	4e	0.6195	0.2442	0.0759	0.080
H(56)	4e	0.4652	0.3045	0.1341	0.065
H(62)	4e	0.5410	0.3583	0.2416	0.090
H(63)	4e	0.5652	0.3128	0.3379	0.114
H(64)	4e	0.4245	0.3657	0.4045	0.132
H(65)	4e	0.2554	0.4500	0.3769	0.109
H(66)	4e	0.2335	0.4926	0.2832	0.086
H(100)	4e	0.8931	0.2581	0.5076	0.178

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Table 3. 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	0.07250(5)	0.20850(3)	0.16950(2)	0.0458(3)	0.0497(3)	0.0533(4)	-0.0025(3)	-0.0017(2)	0.0022(3)
Sn(2)	4e	0.36880(5)	0.46961(3)	0.16780(2)	0.0523(3)	0.0494(3)	0.0474(3)	-0.0020(3)	0.0047(2)	-0.0017(3)
Cl(1)	4e	0.9840(4)	0.3582(3)	0.4570(2)	0.173(4)	0.274(6)	0.170(4)	-0.092(4)	-0.035(3)	0.035(4)
Cl(2)	4e	0.7211(4)	0.3139(2)	0.4665(2)	0.155(3)	0.110(3)	0.155(3)	0.014(2)	-0.033(2)	0.003(2)
Cl(3)	4e	0.8945(4)	0.2030(3)	0.4234(2)	0.231(5)	0.204(5)	0.163(4)	0.070(4)	0.003(3)	-0.054(4)
O(1)	4e	0.1019(5)	0.2840(3)	0.0952(2)	0.062(3)	0.054(3)	0.056(3)	-0.016(3)	-0.005(3)	0.001(3)
O(2)	4e	0.2273(4)	0.3668(3)	0.1444(2)	0.049(3)	0.055(3)	0.062(4)	-0.007(3)	-0.002(3)	0.002(3)
O(3)	4e	0.0513(5)	0.1269(3)	0.2469(2)	0.049(3)	0.056(3)	0.056(3)	0.004(3)	0.005(3)	0.012(3)
O(4)	4e	-0.0214(5)	0.0611(3)	0.3198(2)	0.068(4)	0.062(4)	0.066(4)	0.017(3)	0.019(3)	0.015(3)
C(1)	4e	0.1685(7)	0.3447(5)	0.0988(3)	0.052(5)	0.063(6)	0.044(5)	-0.001(5)	0.001(4)	0.002(5)
C(2)	4e	0.1782(9)	0.3945(5)	0.0460(3)	0.105(7)	0.061(6)	0.057(6)	-0.016(5)	-0.013(5)	0.009(5)
C(3)	4e	-0.0373(7)	0.1082(4)	0.2799(3)	0.052(5)	0.040(5)	0.052(5)	0.006(4)	-0.007(4)	0.007(4)
C(4)	4e	-0.1697(8)	0.1460(6)	0.2728(4)	0.051(5)	0.102(8)	0.098(7)	0.009(5)	0.010(5)	0.033(6)
C(11)	4e	0.2735(7)	0.1721(4)	0.1718(4)	0.048(5)	0.053(5)	0.059(6)	0.003(4)	0.007(4)	0.013(4)
C(12)	4e	0.3542(8)	0.1815(5)	0.2183(4)	0.050(5)	0.090(7)	0.066(6)	0.011(5)	-0.009(4)	0.000(5)
C(13)	4e	0.4832(9)	0.1581(7)	0.2172(4)	0.067(7)	0.124(9)	0.085(8)	0.008(6)	-0.021(6)	0.015(7)
C(14)	4e	0.5290(9)	0.1224(6)	0.1699(5)	0.059(6)	0.101(8)	0.111(1)	0.018(6)	0.013(6)	0.021(8)
C(15)	4e	0.447(1)	0.1117(6)	0.1228(4)	0.090(8)	0.089(7)	0.077(7)	0.010(6)	0.018(6)	0.005(6)
C(16)	4e	0.3153(8)	0.1359(5)	0.1244(4)	0.067(6)	0.072(6)	0.060(6)	0.013(5)	-0.006(5)	0.007(5)
C(21)	4e	-0.0167(7)	0.3014(4)	0.2134(3)	0.060(5)	0.051(5)	0.054(5)	-0.010(4)	0.011(4)	-0.001(4)
C(22)	4e	0.0223(8)	0.3282(6)	0.2666(4)	0.070(6)	0.080(7)	0.075(7)	0.014(5)	-0.009(5)	-0.008(6)
C(23)	4e	-0.042(1)	0.3922(6)	0.2909(4)	0.12(1)	0.083(8)	0.072(7)	-0.009(7)	-0.002(7)	-0.015(6)
C(24)	4e	-0.146(1)	0.4252(6)	0.2639(6)	0.097(9)	0.064(7)	0.121(1)	0.002(6)	0.028(7)	-0.025(7)
C(25)	4e	-0.1832(9)	0.4007(6)	0.2114(5)	0.055(6)	0.094(8)	0.115(9)	0.003(6)	0.005(6)	-0.007(7)
C(26)	4e	-0.1190(8)	0.3411(6)	0.1863(4)	0.065(6)	0.079(7)	0.074(7)	0.015(5)	0.004(5)	-0.010(5)
C(31)	4e	-0.0568(7)	0.1382(5)	0.1158(3)	0.046(5)	0.058(5)	0.058(6)	0.001(4)	0.002(4)	0.002(4)
C(32)	4e	-0.0930(9)	0.0621(5)	0.1312(4)	0.093(7)	0.062(6)	0.062(6)	0.004(5)	-0.002(5)	-0.009(5)
C(33)	4e	-0.173(1)	0.0166(5)	0.0956(5)	0.115(8)	0.060(7)	0.100(8)	-0.010(6)	-0.017(7)	-0.025(6)
C(34)	4e	-0.221(1)	0.0465(7)	0.0448(5)	0.106(8)	0.090(8)	0.091(8)	-0.027(7)	-0.019(7)	-0.021(7)
C(35)	4e	-0.1870(9)	0.1216(6)	0.0290(4)	0.075(6)	0.104(8)	0.059(6)	-0.016(6)	-0.005(5)	-0.009(6)
C(36)	4e	-0.1031(8)	0.1663(5)	0.0644(4)	0.078(6)	0.051(5)	0.074(7)	-0.006(5)	-0.008(5)	-0.004(5)
C(41)	4e	0.2166(8)	0.5493(5)	0.1441(3)	0.075(6)	0.053(6)	0.044(5)	0.005(5)	0.013(4)	-0.002(4)
C(42)	4e	0.2436(9)	0.6206(6)	0.1193(4)	0.094(7)	0.065(6)	0.075(7)	-0.003(6)	0.027(6)	0.008(5)
C(43)	4e	0.140(1)	0.6714(7)	0.1004(5)	0.15(1)	0.097(9)	0.099(9)	0.05(1)	0.024(9)	0.017(7)
C(44)	4e	0.016(1)	0.6492(8)	0.1073(5)	0.11(1)	0.10(1)	0.11(1)	0.06(1)	-0.016(8)	-0.002(8)
C(45)	4e	-0.012(1)	0.5808(8)	0.1318(5)	0.067(7)	0.13(1)	0.11(1)	0.040(8)	-0.008(6)	-0.035(8)
C(46)	4e	0.0862(9)	0.5312(5)	0.1496(4)	0.065(6)	0.077(6)	0.089(7)	0.002(6)	0.008(5)	-0.023(6)
C(51)	4e	0.4987(7)	0.4168(5)	0.1098(3)	0.047(5)	0.057(5)	0.043(5)	0.005(4)	0.011(4)	-0.003(4)
C(52)	4e	0.5748(9)	0.4623(5)	0.0751(4)	0.098(7)	0.054(5)	0.063(6)	-0.005(5)	0.023(5)	0.016(5)
C(53)	4e	0.662(1)	0.4277(6)	0.0386(4)	0.126(9)	0.073(7)	0.076(7)	0.011(7)	0.053(6)	0.010(6)
C(54)	4e	0.6756(9)	0.3466(6)	0.0402(4)	0.098(8)	0.086(7)	0.057(6)	0.025(6)	0.016(5)	-0.003(6)
C(55)	4e	0.6068(9)	0.3007(5)	0.0749(4)	0.084(7)	0.053(6)	0.064(6)	0.007(5)	0.008(5)	0.000(5)
C(56)	4e	0.5167(7)	0.3369(5)	0.1095(3)	0.060(5)	0.051(5)	0.053(5)	0.001(4)	0.005(4)	0.001(4)
C(61)	4e	0.3834(7)	0.4291(5)	0.2523(3)	0.056(5)	0.059(5)	0.045(5)	0.002(4)	-0.001(4)	-0.003(4)
C(62)	4e	0.4812(8)	0.3773(5)	0.2696(4)	0.079(6)	0.089(7)	0.056(6)	0.009(6)	0.003(5)	0.001(5)
C(63)	4e	0.498(1)	0.3506(7)	0.3266(4)	0.103(8)	0.127(9)	0.053(7)	0.035(7)	-0.015(6)	0.012(6)
C(64)	4e	0.414(1)	0.3808(7)	0.3648(5)	0.17(1)	0.092(9)	0.072(8)	-0.007(8)	0.013(8)	0.009(7)
C(65)	4e	0.316(1)	0.4312(6)	0.3490(4)	0.124(9)	0.098(8)	0.052(7)	0.014(7)	0.030(6)	0.021(6)
C(66)	4e	0.3025(8)	0.4554(5)	0.2937(4)	0.077(6)	0.074(6)	0.065(6)	0.005(5)	0.012(5)	-0.002(5)
C(100)	4e	0.874(1)	0.2776(8)	0.4694(5)	0.17(1)	0.13(1)	0.14(1)	0.00(1)	-0.05(1)	0.00(1)

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