Cl(3)	0.5326 (2)	−0.1960 (2)	0.0672 (1)	0.060 (1)
P(1)	0.3507 (2)	0.0788 (1)	0.2215 (1)	0.033 (1)
C(1)	0.1853 (6)	0.1107 (5)	0.1710 (5)	0.035 (2)
C(2)	0.1659 (7)	0.1029 (5)	0.0753 (5)	0.046 (2)
C(3)	0.0429 (7)	0.1285 (6)	0.0355 (5)	0.055 (3)
C(4)	−0.0613 (7)	0.1615 (6)	0.0903 (6)	0.059 (3)
C(5)	−0.0416 (7)	0.1693 (7)	0.1840 (7)	0.068 (3)
C(6)	0.0815 (7)	0.1445 (6)	0.2260 (5)	0.053 (3)
C(7)	0.4505 (6)	0.1928 (5)	0.2236 (4)	0.035 (2)
C(8)	0.4226 (6)	0.2679 (5)	0.1592 (5)	0.042 (2)
C(9)	0.4992 (8)	0.3573 (6)	0.1618 (6)	0.057 (3)
C(10)	0.5988 (8)	0.3685 (7)	0.2269 (6)	0.061 (3)
C(11)	0.6279 (7)	0.2958 (7)	0.2906 (6)	0.059 (3)
C(12)	0.5552 (6)	0.2059 (5)	0.2886 (5)	0.047 (3)
C(13)	0.3355 (6)	0.0396 (5)	0.3417 (5)	0.037 (2)
C(14)	0.2941 (7)	0.1108 (5)	0.4070 (5)	0.047 (3)
C(15)	0.2750 (8)	0.0835 (6)	0.4981 (5)	0.059 (3)
C(16)	0.2968 (8)	−0.0149 (7)	0.5257 (5)	0.060 (3)
C(17)	0.3386 (8)	−0.0850 (6)	0.4632 (5)	0.057 (3)
C(18)	0.3576 (7)	−0.0581 (5)	0.3705 (5)	0.047 (2)

Table 2. *Geometric parameters* (Å, °)

Au(1)—Cl(1)	2.278 (2)	Au(1)—Cl(2)	2.287 (2)
Au(1)—Cl(3)	2.347 (2)	Au(1)—P(1)	2.329 (2)
P(1)—C(1)	1.828 (6)	P(1)—C(7)	1.818 (6)
P(1)—C(13)	1.817 (7)	C(1)—C(2)	1.392 (10)
C(1)—C(6)	1.382 (10)	C(2)—C(3)	1.379 (10)
C(3)—C(4)	1.379 (11)	C(4)—C(5)	1.364 (14)
C(5)—C(6)	1.390 (11)	C(7)—C(8)	1.392 (9)
C(7)—C(12)	1.394 (9)	C(8)—C(9)	1.418 (10)
C(9)—C(10)	1.357 (12)	C(10)—C(11)	1.366 (12)
C(11)—C(12)	1.402 (11)	C(13)—C(14)	1.404 (10)
C(13)—C(18)	1.389 (10)	C(14)—C(15)	1.378 (11)
C(15)—C(16)	1.392 (12)	C(16)—C(17)	1.368 (11)
C(17)—C(18)	1.398 (11)		
Cl(1)—Au(1)—Cl(2)	178.4 (1)	Cl(1)—Au(1)—Cl(3)	90.9 (1)
Cl(2)—Au(1)—Cl(3)	90.5 (1)	Cl(1)—Au(1)—P(1)	91.9 (1)
Cl(2)—Au(1)—P(1)	86.6 (1)	Cl(3)—Au(1)—P(1)	175.5 (1)
Au(1)—P(1)—C(1)	109.8 (2)	Au(1)—P(1)—C(7)	115.4 (2)
C(1)—P(1)—C(7)	107.0 (3)	Au(1)—P(1)—C(13)	107.3 (2)
C(1)—P(1)—C(13)	111.1 (3)	C(7)—P(1)—C(13)	106.2 (3)
P(1)—C(1)—C(2)	119.0 (5)	P(1)—C(1)—C(6)	121.0 (5)
C(2)—C(1)—C(6)	120.0 (6)	C(1)—C(2)—C(3)	120.0 (7)
C(2)—C(3)—C(4)	120.2 (7)	C(3)—C(4)—C(5)	119.6 (7)
C(4)—C(5)—C(6)	121.5 (8)	C(1)—C(6)—C(5)	118.8 (7)
P(1)—C(7)—C(8)	119.5 (5)	P(1)—C(7)—C(12)	120.9 (5)
C(8)—C(7)—C(12)	119.6 (6)	C(7)—C(8)—C(9)	119.5 (6)
C(8)—C(9)—C(10)	119.5 (7)	C(9)—C(10)—C(11)	121.9 (8)
C(10)—C(11)—C(12)	119.7 (7)	C(7)—C(12)—C(11)	119.7 (7)
P(1)—C(13)—C(14)	118.0 (5)	P(1)—C(13)—C(18)	122.8 (5)
C(14)—C(13)—C(18)	119.1 (6)	C(13)—C(14)—C(15)	120.2 (7)
C(14)—C(15)—C(16)	119.9 (7)	C(15)—C(16)—C(17)	120.7 (7)
C(16)—C(17)—C(18)	119.8 (7)	C(13)—C(18)—C(17)	120.3 (7)

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71402 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1064]

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Structure of Dichlorobis(μ-hydroxo)-bis(μ_3-oxo)octaphenyltetratin(IV), $[Sn_4Cl_2(O)_2(OH)_2(C_6H_5)_8]$

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Abstract

The structure of the title compound, dichloro-1κCl,3κCl-di-μ-hydroxo-1:2κ^2O;3:4κ^2O-di-μ_3-oxo-1:2:4κ^3O;2:3:4κ^3O-octaphenyl-1κ^2C,2κ^2C,3κ^2C,-4κ^2C-*quadro*-tetratin(IV), consists of an almost planar array of four Sn^{IV} atoms bridged by two O^{2-} and two OH^- ligands. Each Sn atom is bonded to two phenyl groups and the two terminal Sn atoms of the array are bonded to Cl^- ligands. In this way, each Sn atom possesses a rather distorted trigonal bipyramidal coordination geometry.

Comment

$[Sn(Cl)Ph_2(\mu\text{-}O)(\mu\text{-}OH)SnPh_2]_2$ was obtained as a contaminant in the preparation of $[Ph_2SnCl\{\mu\text{-}CH_2\text{-}P(O)Ph_2\}]_2$ from $[Ph_2SnCl_2]$ and $[Li\{CH_2P(O)Ph_2\}]$, believed to occur due to the presence of traces of

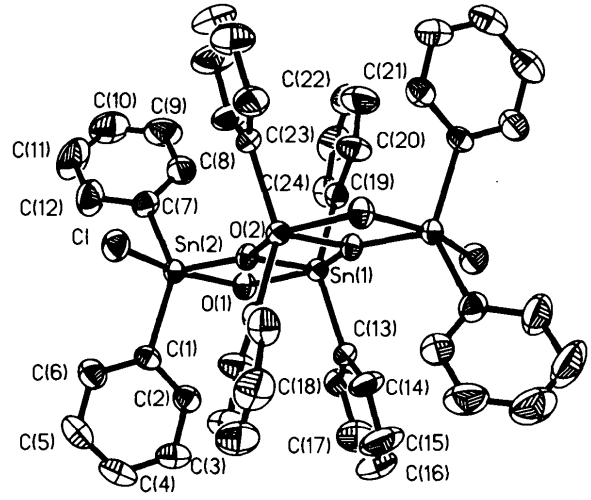

Fig. 1. View of $[Sn(Cl)Ph_2(\mu\text{-}O)(\mu\text{-}OH)SnPh_2]_2$. H atoms have been omitted; thermal ellipsoids have been drawn at the 50% probability level.

water in the reaction mixture. The structure of $[Sn(Cl)Ph_2(\mu\text{-}O)(\mu\text{-}OH)SnPh_2]_2$ is very similar to that obtained for the solvated material (Vollano, Day & Holmes, 1984). The structures of $[SnCl(CH_2SiMe_3)_2(\mu\text{-}O)(\mu\text{-}OH)Sn(CH_2SiMe_3)_2]_2$, $[SnCl(CHMe_2)_2(\mu\text{-}O)(\mu\text{-}OH)Sn(CHMe_2)_2]_2$ (Puff, Bung, Friedrichs & Jansen, 1983) and $[Ph_2SnCl(\mu\text{-}O)(\mu\text{-}OH)SnPh_2]_2.2C_3H_7NO$ (Tiekink, 1991) have also been determined. A view of the molecule is shown in Fig. 1.

Experimental

Crystal data

$[Sn_4Cl_2(O)_2(OH)_2(C_6H_5)_8]$	D_x = 1.76 Mg m^{-3}
M_r = 1228.52	Mo $K\alpha$ radiation
Triclinic	λ = 0.71073 Å
$P\bar{1}$	Cell parameters from 20 reflections
a = 10.295 (3) Å	θ = 12.5–15°
b = 10.791 (3) Å	μ = 2.302 mm^{-1}
c = 11.827 (4) Å	T = 293 K
α = 77.74 (3)°	Prism
β = 66.49 (2)°	0.6 × 0.4 × 0.2 mm
γ = 75.63 (2)°	Colorless
V = 1157.6 (6) Å^3	
Z = 1	

Data collection

Siemens *R3m/E* diffractometer	R_{int} = 0.0345
Wyckoff scans	θ_{max} = 22.5°
Absorption correction: empirical	h = 0 → 11
T_{min} = 0.702, T_{max} = 0.955	k = −11 → 11
3283 measured reflections	l = −12 → 12
3002 independent reflections	3 standard reflections monitored every 97 reflections
2534 observed reflections [$F_o^2 > 3\sigma(F_o)^2$]	intensity variation: <1%

Refinement

Refinement on F	$w = [\sigma^2(F_o) + 0.0005F_o^2]^{-1}$
R = 0.0237	$(\Delta/\sigma)_{max}$ = 0.006
wR = 0.0312	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
S = 1.080	$\Delta\rho_{min}$ = −0.90 e Å^{-3}
2534 reflections	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
262 parameters	
H-atom parameters not refined	

Computer programs used for the structure determination: *SHELXTL* (Sheldrick, 1985).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Sn1	0.8865 (1)	0.4478 (1)	0.9600 (1)	0.028 (1)
Sn2	1.0262 (1)	0.2050 (1)	1.1363 (1)	0.031 (1)
Cl	1.1980 (1)	0.2372 (1)	1.2218 (1)	0.048 (1)
O1	0.8802 (3)	0.2467 (3)	1.0353 (3)	0.036 (1)
O2	1.0204 (3)	0.3910 (2)	1.0587 (2)	0.031 (1)
C1	1.1809 (4)	0.0726 (4)	1.0156 (4)	0.033 (2)
C2	1.1868 (5)	0.0810 (4)	0.8948 (4)	0.043 (2)
C3	1.2972 (5)	0.0083 (5)	0.8092 (4)	0.051 (2)
C4	1.4008 (5)	−0.0784 (5)	0.8463 (5)	0.054 (2)
C5	1.3941 (5)	−0.0913 (5)	0.9661 (5)	0.056 (3)
C6	1.2854 (5)	−0.0144 (4)	1.0513 (5)	0.049 (2)
C7	0.8599 (5)	0.1678 (4)	1.3110 (4)	0.041 (2)
C8	0.7235 (5)	0.2374 (5)	1.3383 (4)	0.055 (2)
C9	0.6145 (6)	0.2059 (6)	1.4483 (5)	0.077 (3)
C10	0.6431 (7)	0.1042 (6)	1.5319 (5)	0.082 (3)
C11	0.7772 (7)	0.0368 (7)	1.5079 (5)	0.094 (4)
C12	0.8880 (6)	0.0686 (6)	1.3967 (5)	0.070 (3)
C13	0.9858 (4)	0.4068 (4)	0.7741 (4)	0.036 (2)
C14	1.1020 (6)	0.4645 (5)	0.6915 (4)	0.058 (2)
C15	1.1735 (7)	0.4326 (7)	0.5728 (5)	0.089 (4)
C16	1.1282 (8)	0.3473 (7)	0.5336 (6)	0.094 (4)
C17	1.0152 (8)	0.2893 (6)	0.6122 (6)	0.081 (4)
C18	0.9452 (6)	0.3169 (5)	0.7331 (5)	0.055 (2)
C19	0.6742 (4)	0.5171 (4)	1.0797 (4)	0.035 (2)
C20	0.6502 (5)	0.6266 (5)	1.1331 (4)	0.054 (2)
C21	0.5169 (7)	0.6652 (6)	1.2225 (5)	0.078 (3)
C22	0.4112 (6)	0.5977 (7)	1.2578 (5)	0.077 (3)
C23	0.4314 (5)	0.4910 (7)	1.2045 (5)	0.068 (3)
C24	0.5648 (5)	0.4496 (5)	1.1152 (4)	0.048 (2)

Table 2. *Geometric parameters* (Å, °)

Sn1—O1	2.171 (3)	Sn1—O2	2.048 (3)
Sn1—C13	2.113 (4)	Sn1—C19	2.120 (3)
Sn1—O2a	2.117 (3)	Sn2—Cl	2.480 (2)
Sn2—O1	2.180 (3)	Sn2—O2	2.020 (2)
Sn2—C1	2.129 (4)	Sn2—C7	2.125 (4)
O1—Sn1—O2	72.3 (1)	O1—Sn1—C13	93.1 (1)
O2—Sn1—C13	113.9 (1)	O1—Sn1—C19	94.8 (1)
O2—Sn1—C19	109.7 (2)	C13—Sn1—C19	136.0 (2)
O1—Sn1—O2a	145.8 (1)	O2—Sn1—O2a	73.6 (1)
C13—Sn1—O2a	99.0 (1)	C19—Sn1—O2a	98.2 (1)
Cl—Sn2—O1	160.0 (1)	Cl—Sn2—O2	87.3 (1)
O1—Sn2—O2	72.6 (1)	Cl—Sn2—C1	94.3 (1)
O1—Sn2—C1	93.6 (2)	O2—Sn2—C1	113.6 (1)
Cl—Sn2—C7	96.1 (2)	O1—Sn2—C7	93.1 (2)
O2—Sn2—C7	116.4 (1)	C1—Sn2—C7	129.3 (2)
Sn1—O1—Sn2	102.3 (1)	Sn1—O2—Sn2	112.8 (2)
Sn1—O2—Sn1a	106.4 (1)	Sn2—O2—Sn1a	140.8 (2)

Symmetry code: 2 − x, 1 − y, 2 − z.

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