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Rhombohedral Chlorotriphenyltin

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Abstract

The Sn atoms in the two independent molecules of rhombohedral chlorotriphenyltin, $[SnCl(C_6H_5)_3]$, both show tetrahedral coordination.

Comment

This rhombohedral modification of chlorotriphenyltin shows no new or unusual features compared with the monoclinic modification, which also has two independent but structurally similar tetrahedral molecules in the unit cell (Tse, Lee & Gabe, 1986). In the title complex the molecule containing Sn2 and Cl2 has exact threefold symmetry.

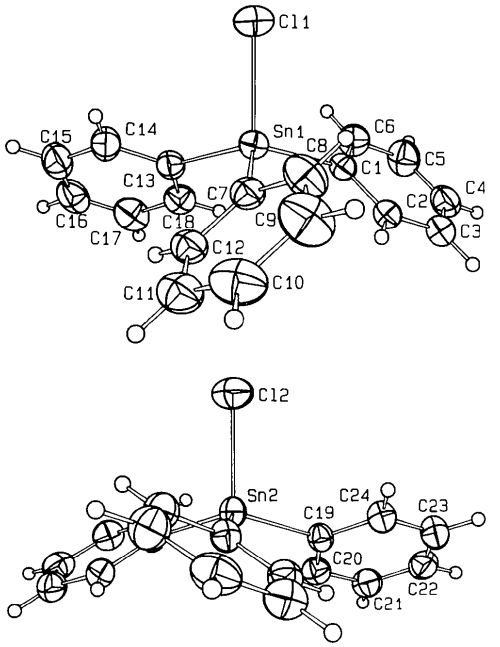
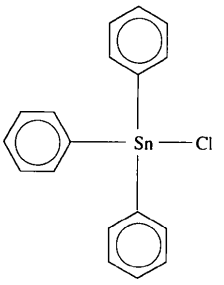


Fig. 1. Atomic labelling scheme for the two crystallographically independent molecules of chlorotriphenyltin. Displacement ellipsoids are plotted at the 30% probability level.



(I)

Experimental

This modification of triphenyltin chloride was obtained in an unsuccessful attempt at synthesizing the 1/1 complex with 2,2′-bipyridine *N*,*N*′-dioxide. The reagents in equimolar amounts were heated in a small volume of ethanol; slow cooling of the solution returned the starting organotin halide in the rhombohedral modification.

Crystal data

$[SnCl(C_6H_5)_3]$
M_r = 385.44
Trigonal
$R\bar{3}$ (hexagonal axes)
a = 24.4935 (4) Å
c = 19.1219 (6) Å
V = 9934.9 (4) Å^3
Z = 24
D_x = 1.546 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 14–15°
μ = 1.692 mm^{-1}
T = 298 K
Cube
0.44 × 0.44 × 0.44 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scans (North, Phillips & Mathews, 1968)
T_{min} = 0.91, T_{max} = 1.00
4189 measured reflections
3887 independent reflections
2853 observed reflections [$I > 2\sigma(I)$]
R_{int} = 0.0174
θ_{max} = 24.97°
h = 0 → 25
k = 0 → 25
l = −22 → 22
3 standard reflections
frequency: 60 min
intensity decay: 0.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0344
$wR(F^2)$ = 0.0766
S = 1.088
3887 reflections
321 parameters
H-atoms were located and refined isotropically
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 6.3034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement 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	0.35981 (2)	0.28419 (2)	0.61695 (2)	0.06046 (12)
Cl1	0.38740 (8)	0.38490 (6)	0.57433 (8)	0.0994 (4)
C1	0.3657 (2)	0.2333 (2)	0.5305 (2)	0.0548 (9)
C2	0.4041 (2)	0.2074 (2)	0.5349 (2)	0.0592 (10)
C3	0.4066 (3)	0.1709 (2)	0.4814 (3)	0.0760 (14)
C4	0.3707 (3)	0.1599 (3)	0.4233 (3)	0.086 (2)
C5	0.3326 (3)	0.1849 (3)	0.4172 (3)	0.094 (2)
C6	0.3302 (3)	0.2218 (3)	0.4702 (3)	0.0803 (15)
C7	0.4288 (2)	0.3000 (2)	0.6938 (2)	0.0610 (10)
C8	0.4919 (3)	0.3312 (2)	0.6781 (3)	0.087 (2)
C9	0.5361 (3)	0.3395 (3)	0.7280 (4)	0.104 (2)
C10	0.5166 (3)	0.3166 (3)	0.7940 (4)	0.100 (2)
C11	0.4551 (3)	0.2855 (2)	0.8106 (3)	0.0826 (15)
C12	0.4111 (3)	0.2769 (2)	0.7606 (2)	0.0674 (12)
C13	0.2690 (2)	0.2469 (2)	0.6608 (2)	0.0613 (10)
C14	0.2566 (3)	0.2804 (3)	0.7119 (3)	0.0780 (13)
C15	0.1982 (3)	0.2536 (4)	0.7438 (3)	0.093 (2)
C16	0.1525 (3)	0.1940 (4)	0.7256 (3)	0.094 (2)
C17	0.1633 (3)	0.1608 (3)	0.6763 (3)	0.090 (2)
C18	0.2210 (2)	0.1872 (2)	0.6437 (3)	0.0733 (13)
Sn2	2/3	1/3	0.47166 (3)	0.05609 (15)
Cl2	2/3	1/3	0.59582 (11)	0.0913 (7)
C19	0.6239 (2)	0.2369 (2)	0.4450 (2)	0.0534 (9)
C20	0.5680 (2)	0.2074 (2)	0.4074 (2)	0.0647 (11)
C21	0.5391 (2)	0.1441 (2)	0.3919 (3)	0.0751 (13)
C22	0.5659 (3)	0.1096 (2)	0.4138 (3)	0.0804 (14)
C23	0.6214 (3)	0.1380 (3)	0.4502 (3)	0.083 (2)
C24	0.6504 (2)	0.2012 (2)	0.4658 (2)	0.0685 (12)

Table 2. *Selected geometric parameters* (Å, °)

Sn1—C13	2.109 (4)	Sn1—Cl1	2.3535 (12)
Sn1—C1	2.118 (4)	Sn2—C19	2.112 (4)
Sn1—C7	2.124 (4)	Sn2—Cl2	2.374 (2)
C13—Sn1—C1	115.0 (2)	C8—C7—Sn1	121.4 (3)
C13—Sn1—C7	112.0 (2)	C12—C7—Sn1	120.6 (3)
C1—Sn1—C7	111.5 (2)	C18—C13—C14	117.6 (4)
C13—Sn1—Cl1	106.22 (12)	C18—C13—Sn1	121.3 (3)
C1—Sn1—Cl1	106.13 (11)	C14—C13—Sn1	120.9 (4)
C7—Sn1—Cl1	105.27 (11)	C19—Sn2—C19^i	114.36 (8)
C2—C1—C6	117.4 (4)	C19—Sn2—Cl2	103.97 (10)
C2—C1—Sn1	119.1 (3)	C24—C19—C20	118.2 (4)
C6—C1—Sn1	123.3 (3)	C24—C19—Sn2	120.7 (3)
C8—C7—C12	117.9 (4)	C20—C19—Sn2	121.1 (3)

Symmetry code: (i) $1-y, x-y, z$.

Data collection: *CAD-4 VAX/PC* (Enraf–Nonius, 1988). Cell refinement: *CAD-4 VAX/PC*. Data reduction: *Xtal3.0* (Hall & Stewart, 1990). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1190). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(cytosinium) Tetrachlorodimethylstannate(IV)

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Abstract

The structure of the title compound, bis(4-amino-2-oxo-1,2-dihydropyrimidinium) tetrachlorodimethylstannate(IV), $(C_4H_6N_3O)_2[SnCl_4(CH_3)_2]$, consists of discrete $C_4H_6N_3O^+$ (cytosinium) cations and $[SnCl_4(CH_3)_2]^{2-}$ anions in which the Sn atom is six-coordinate *trans*-octahedral. The crystal packing of the ionic complex is stabilized by intermolecular N—H···Cl bonds between the anions and neighbouring cytosinium cations.

Comment

The antitumor activity of organotin(IV) complexes is known (Kabanos, Keramidas, Mentzafos, Russo, Terzis & Tsangaris, 1992). Because of interest in the possible interaction of these compounds with the constituents of nucleic acids, we report here the crystal structure of the title compound, $(C_4H_6N_3O)_2[SnCl_4(CH_3)_2]$, (I).