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Bis[1,2-bis(diphenylphosphino)ethane]silver(I) bis(trifluoroacetato)triphenylstannate(IV)

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Key indicators

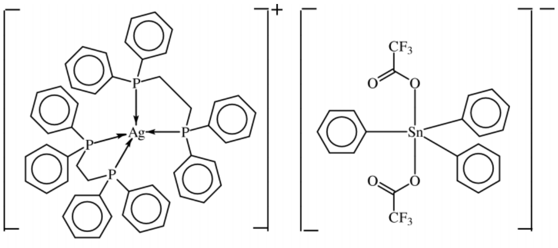
Single-crystal X-ray study
T = 168 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.042
wR factor = 0.122
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title compound, $[Ag(C_{26}H_{24}P_2)_2][Sn(C_2O_2F_3)_2(C_6H_5)_3]$, consists of discrete tetrahedral $[[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]_2Ag]^+$ cations and *trans*-C_3SnO_2 trigonal bipyramidal $[(C_6H_5)_3Sn(O_2CCF_3)_2]^-$ anions.

Comment

One strategy for improving the water solubility of fungicidal triorganotin carboxylates involves the addition of a carboxylate anion to the compound to furnish a di(carboxylato)triorganostannate, whose negative charge is balanced by an ammonium cation. The first example of such an ammonium stannate has the tetramethylammonium cation as counterion (Ng & Kumar Das, 1997*a*,*b*); other ammonium stannates have also been synthesized (Ng, 1999; Ng & Hook, 1999). In addition to these ammonium salts, the extremely large tetrakis(triphenylphosphine)silver(I) cation has also been used for this purpose; the salt of bis(trifluoroacetato)triphenylstannate consists of discrete tetrahedral cations and five-coordinate *trans*-trigonal bipyramidal anions. The structure is both twinned and disordered [molecule *a*: Ag—P 2.563 (4)/2.717 (2) Å and Sn—O 2.234 (6)/2.236 (5) Å; molecule *b*: Ag—P 2.632 (2)/2.768 (3) Å and Sn—O 2.234 (6)/2.235 (6) Å] (Ng & Rae, 2003). The bis(trifluoroacetato)triphenylstannate anion, as isolated in the present bis[1,2-bis(diphenylphosphino)ethane]silver salt, (I), (see Scheme) represents yet another uncommon example of such a bimetallic compound.



(I)

The Ag atom in the cation (Fig. 1) is chelated by the phosphine ligands, which bind in a nearly isobidentate manner [Ag—P 2.488 (1)/2.520 (1) and 2.495 (1)/2.517 (1) Å] to give rise to a tetrahedral environment for the Ag atom (Fig. 1). The Ag—P distances are similar to those found in the bis[1,2-bis(diphenylphosphino)ethene)]silver salt of the dinitratotriphenylstannate anion (Franzoni *et al.*, 1988); the bite angles in the title cation are similar to those [83.9 (1) and 84.1 (1)°] found in this complex, which has a CH═CH fragment. In the bis(trifluoroacetato)triphenylstannate anion (Fig. 2), the O—Sn—O skeleton is nearly linear [Sn—O 2.213 (3)/2.250 (3) Å; O—Sn—O 177.6 (1)°]. The trigonal bipyramidal geometry of the Sn atom is distorted by the two double-bond carbonyl O

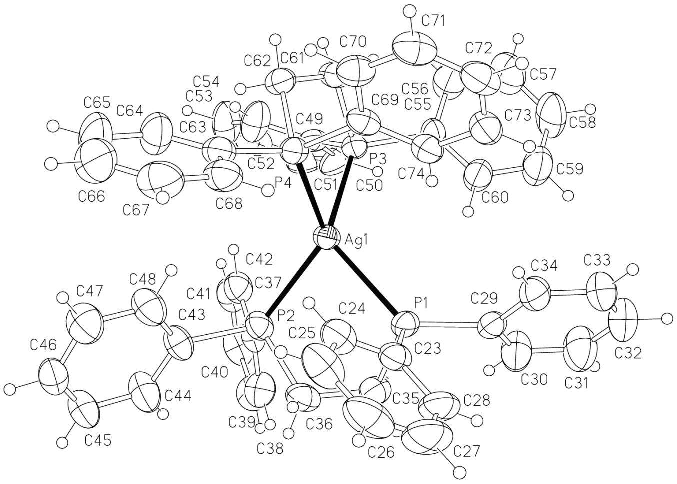


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title cation, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

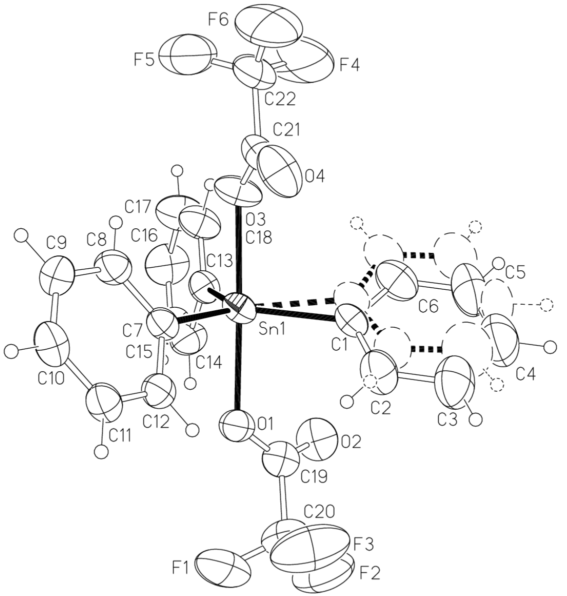


Figure 2
*ORTEP*II (Johnson, 1976) plot of the title anion, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. The disorder in one of the phenyl rings is shown.

atoms at distances of *ca* 3.5 Å. The cations and anions exist as discrete entities in the unit cell (Fig. 3).

Experimental

The synthesis was carried out on a mmol scale. The cationic entity was synthesized from the reaction of silver trifluoroacetate and 2 equivalents of 1,2-bis(diphenylphosphine)ethane in acetone, to yield bis[bis-1,2-(diphenylphosphino)ethane)]silver trifluoroacetate *in situ*. The anionic entity was synthesized from the reaction of triphenyltin hydroxide and trifluoroacetic acid in the same solvent. The two reagents were mixed and the solution briefly heated. Large colorless crystals of the silver stannate separated from the cool solution when it was set aside for a day.

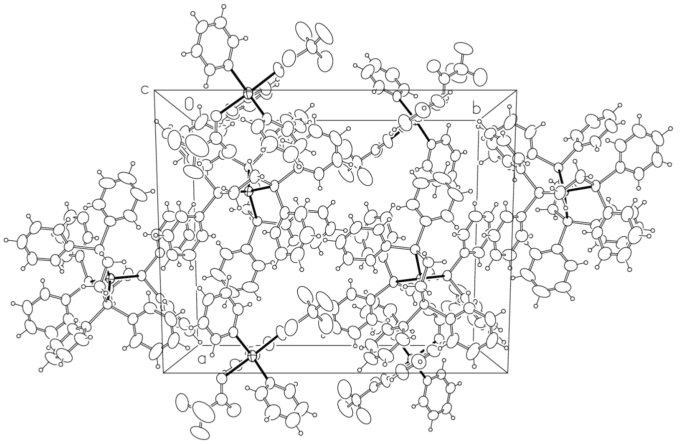


Figure 3
*ORTEP*II (Johnson, 1976) plot of the packing.

Crystal data

$[Ag(C_{26}H_{24}P_2)_2]$-
$[Sn(C_2O_2F_3)_2(C_6H_5)_3]$
$M_r = 1480.68$
Monoclinic, $P2_1/n$
$a = 15.988$ (1) Å
$b = 19.115$ (1) Å
$c = 23.875$ (1) Å
$\beta = 107.279$ (1)°
$V = 6966.9$ (7) Å^3
$Z = 4$

$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7800 reflections
$\theta = 1.7$–26.5°
$\mu = 0.80$ mm^{-1}
$T = 168$ (2) K
Block, colorless
0.50 × 0.50 × 0.36 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.518$, $T_{\max} = 0.742$
85582 measured reflections

14277 independent reflections
10420 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 26.5°$
$h = -20 \rightarrow 19$
$k = -23 \rightarrow 21$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.122$
$S = 1.06$
14277 reflections
842 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 13.3659P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 2.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.62$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.140 (4)	Sn1—O3	2.213 (3)
Sn1—C1′	2.125 (5)	Ag1—P1	2.520 (1)
Sn1—C7	2.133 (4)	Ag1—P2	2.488 (1)
Sn1—C13	2.156 (4)	Ag1—P3	2.495 (1)
Sn1—O1	2.250 (3)	Ag1—P4	2.517 (1)
C1—Sn1—C7	120.5 (2)	C7—Sn1—O3	91.4 (1)
C1—Sn1—C13	118.8 (2)	C13—Sn1—O3	86.1 (1)
C1—Sn1—O1	85.9 (3)	C13—Sn1—O1	95.0 (1)
C1—Sn1—O3	95.5 (3)	O1—Sn1—O3	177.6 (1)
C1′—Sn1—C7	127.3 (5)	P1—Ag1—P2	84.7 (1)
C1′—Sn1—C13	111.6 (5)	P1—Ag1—P3	124.3 (1)
C1′—Sn1—O1	96.1 (4)	P1—Ag1—P4	118.5 (1)
C1′—Sn1—O3	85.5 (4)	P2—Ag1—P3	125.2 (1)
C7—Sn1—C13	120.7 (2)	P2—Ag1—P4	124.7 (1)
C7—Sn1—O1	86.2 (1)	P3—Ag1—P4	84.2 (1)

One of the Sn-bound phenyl rings is disordered over two sites; the disordered rings were refined as rigid hexagons. The Sn1—C1 and Sn1—C1′ bond distances were restrained to be approximately equal. Additionally, the C atoms of the rings were restrained to be approximately isotropic. All H atoms were positioned geometrically, and they were allowed to ride on their parent atoms, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C). The final difference Fourier map had a peak of 2.2 e Å^{-3} at 1.4 Å from the P2 atom and 2.5 Å from the Ag1 atom, but it was otherwise featureless. The calculations on the low-temperature diffraction intensities from another crystal converged to $R = 0.048$ for 10599 $I > 2\sigma(I)$ reflections, but the difference map showed a peak of 1.9 e Å^{-3} at 3 Å from the H35*b* atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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