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Key indicators

Single-crystal X-ray study T = 295 KMean σ (C–C) = 0.007 Å R factor = 0.046 wR factor = 0.147 Data-to-parameter ratio = 17.3

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

catena-Poly[[(trifluoroacetato- κO)silver(I)]- μ -1,2-bis(diphenylphosphino)ethane- $\kappa^2 P:P'$]

In polymeric $[Ag(C_2F_3O_2)(C_{26}H_{24}P_2)]_n$, the carboxylate is monodentate to silver, and the two diphosphine ligands that occupy different positions of $\overline{1}$ site symmetry link the $Ag(C_2O_2F_3)$ units into a chain. The Ag atom shows trigonalplanar coordination. Received 8 November 2005 Accepted 11 November 2005 Online 19 November 2005

Comment

Silver(I) acetate, when reacted with triphenylphosphine, affords adducts with different metal-ligand stoichiometries, whereas silver(I) trifluoroacetate yields only the 1:2 adduct. The silver is four-coordinate in the trifluoroacetate-chelated monomeric adduct (Ng, 1998). The flexible diphosphine 1,6bis(diphenylphosphino)hexane furnishes a 1:3 adduct, and the fourth coordination site of the tetrahedral environment arises from coordination by a monodentate carboxylate (Brandys & Puddephatt, 2002). The smaller 1,2-bis(diphenylphosphino)ethane donor ligand in the title compound, (I), does not function in a chelating mode. The two independent ligands lie on inversion sites so that the manner of bridging leads to a chain motif (Fig. 1). On the other hand, the rigid diphosphine 1,2-bis(diphenylphosphino)ethene, which also exists in a 1:1 adduct, has both the phosphine ligand and the trifluoroacetate group functioning in a bridging mode (Brandys & Puddephatt, 2002).



Experimental

Silver trifluoroacetate (11 mg, 0.05 mmol) dissolved in methanol (3 ml) was mixed with 1,2-bis(diphenylphosphino)ethane (20 mg, 0.05 mmol) dissolved in DMF (3 ml) to give a yellow solution. The solution was filtered and then layered with diethyl ether. Colorless crystals were obtained after several days.

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metal-organic papers

Z = 2

 $D_x = 1.537 \text{ Mg m}^{-3}$

Cell parameters from 870

 $0.48 \times 0.42 \times 0.12 \text{ mm}$

5624 independent reflections

 $w = 1/[\sigma^2(F_o^2) + (0.0953P)^2 + 0.9973P]$ where $P = (F_o^2 + 2F_c^2)/3$

4418 reflections with $I > 2\sigma(I)$

Mo $K\alpha$ radiation

reflections

 $\begin{array}{l} \theta = 2.5 {-} 26.8^{\circ} \\ \mu = 0.92 \ \mathrm{mm}^{-1} \end{array}$

T = 295 (2) K

Plate, colorless

 $R_{\rm int} = 0.021$

 $\theta_{\rm max} = 27.0^{\circ}$

 $h = -11 \rightarrow 12$

 $k = -14 \rightarrow 14$

 $l = -13 \rightarrow 16$

 $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 1.64 \text{ e } \text{\AA}^{-3}$

 $\Delta \rho_{\rm min} = -0.75 \text{ e } \text{\AA}^{-3}$

Crystal data

 $\begin{bmatrix} Ag(C_2F_3O_2)(C_{26}H_{24}P_2) \end{bmatrix} \\ M_r = 619.28 \\ \text{Triclinic, } P\overline{1} \\ a = 10.105 (1) \text{ Å} \\ b = 11.095 (2) \text{ Å} \\ c = 12.677 (2) \text{ Å} \\ \alpha = 84.697 (2)^{\circ} \\ \beta = 79.043 (2)^{\circ} \\ \gamma = 73.712 (2)^{\circ} \\ V = 1338.1 (3) \text{ Å}^3$

Data collection

Bruker SMART area-detector diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{min} = 0.667, T_{max} = 0.898$ 9445 measured reflections

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.147$
S = 1.01
5624 reflections
325 parameters
H-atom parameters constrained

Table 1

Selected geometric parameters (Å, °).

Ag1-01	2.392 (4)	Ag1-P2	2.428 (1)
Ag1-P1	2.424 (1)		
O1-Ag1-P1	112.2 (2)	P1-Ag1-P2	134.97 (3)
O1-Ag1-P2	112.2 (2)	-	

The aromatic C–C distances were restrained to 1.390 (5) Å and the aliphatic C–C distances to 1.540 (5) Å. H atoms were placed at calculated positions (C–H_{aromatic} = 0.93, C–H_{aliphatic} = 0.97 Å) and were included in the refinement in the riding-model approximation with U_{iso} (H) set to $1.2U_{eq}$ (C). The displacement parameters of the O and F atoms were restrained to a nearly isotropic behavior. The final Fourier map had a large peak about 1.86 Å from F2, but the electron density could not be modeled as water. The electron density was about 2 Å from its symmetry-related equivalent. Furthermore, the solvent-accessible void, as calculated by *PLATON* (Spek, 2003), is too small to accommodate water, and neither does the center of the void coincide with the peak. Additionally, the presence of water was ruled out by the absence of the characteristic broad peak at 3500 cm^{-1} in the IR spectrum of the bulk crystals.



Figure 1

ORTEPII (Johnson, 1976) plot of a portion of the polymeric chain of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii. [Symmetry codes: (i) 1 - x, 1 - y, -z; (ii) -x, 1 - y, 1 - z.]

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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References

Brandys, M. C. & Puddephatt, R. J. (2002). J. Am. Chem. Soc. 124, 3946–3950.Bruker (2000). SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

- Ng, S. W. (1998). Acta Cryst. C54, 743-744.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Spek, A. L. (2003). J. Appl. Cryst. 36, 7-13.