# metal-organic papers

## catena-Poly[[(tetrafluoroborato-κF)silver(I)]-μ-triphenylphosphine-κ²P:C³]

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### Key indicators

Single-crystal X-ray study
$T$ = 150 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.028
$wR$ factor = 0.072
Data-to-parameter ratio = 22.6

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

The title compound, $[Ag(BF_4)(C_{18}H_{15}P)]_n$, crystallizes from dichloromethane–pentane as a one-dimensional coordination polymer in which the Ag atom is bound to a phosphine P atom, one F atom of tetrafluoroborate and one C atom of a neighbouring triphenylphosphine ligand.

### Comment

Complexes of silver in which close metal–arene interactions are present in the solid state are not uncommon, with the first example reported by Smith & Rundle (1958). Typically, in such complexes, the silver is partnered with weakly or non-coordinating anions such as trifluoromethanesulfonate or perchlorate. On the other hand, there have been few reports of solid state structures of silver complexes which contain bound tetrafluoroborate.



**(I)**
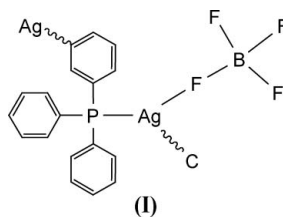
We have previously described (tertiary phosphine)silver complexes of functionalized 1-*closo*-carborane anions (Patmore *et al.*, 2002; Clarke *et al.*, 2004). Whilst attempting to prepare one such complex from silver tetrafluoroborate and $[(PPh_3)_2Rh(nbd)]\cdot CB_{11}H_7Et_5$ (Molinos *et al.*, 2005), colourless single crystals suitable for an X-ray diffraction experiment were obtained. The crystals were determined to be the title complex, (I), and the results of the diffraction study are described below.

In (I) (Fig. 1), the coordination of the silver is quasi-trigonal, the silver bonding to P, F1 and C3$^i$ [symmetry code: (i) $\frac{3}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$], with the silver having only slight deviation from the P—F—C ligand plane [0.0672 (7) Å]. The Ag—C3$^i$ and Ag—F1 distances are long (Table 1), but are consistent with bonding interactions, and the coordination of C3$^i$ results in a one-dimensional coordination polymer. As expected, the coordination of F1 results in a B—F1 distance greater than the other B—F distances.

There are two other Ag$\cdots$F contacts within van der Waals radii. An Ag$\cdots$F2 contact is accommodated by a small Ag—F1—B—F2 torsion angle and a reduced F1—B—F2 angle. The effect of this close contact is also seen in an increased P—Ag—F1 angle relative to P—Ag—C3$^i$ and F1—Ag—C3$^i$. Finally, an Ag$\cdots$F contact occurs between Ag and F3$^{ii}$ [symmetry code:

(ii) $1 - x$, $-y$, $-z$] in a pairwise manner, with a matching contact between the symmetry-related Ag$^{ii}$ and F3 (Fig. 2).

## Experimental

A solution containing equimolar quantities of silver tetrafluoroborate and [(PPh$_3$)$_2$Rh(nbd)]·CB$_{11}$H$_7$Et$_5$ (Molinos *et al.*, 2005) in dichloromethane was layered with pentanes and held at 278 K for one week to crystallize. A crystal of (I) suitable for a single-crystal X-ray diffraction study was selected directly from the sample.

### Crystal data

| | |
|---|---|
| [Ag(BF$_4$)(C$_{18}$H$_{15}$P)] | $Z = 4$ |
| $M_r = 456.95$ | $D_x = 1.733$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 12.0606$ (1) Å | $\mu = 1.28$ mm$^{-1}$ |
| $b = 11.2379$ (1) Å | $T = 150$ (2) K |
| $c = 12.9254$ (1) Å | Block, colourless |
| $\beta = 90.0093$ (7)° | $0.33 \times 0.25 \times 0.18$ mm |
| $V = 1751.85$ (3) Å$^3$ | |

### Data collection

| | |
|---|---|
| Nonius KappaCCD diffractometer | 31041 measured reflections |
| $\varphi$ and $\omega$ scans | 5109 independent reflections |
| Absorption correction: multi-scan | 4717 reflections with $I > 2\sigma(I)$ |
| ($SORTAV$; Blessing, 1995) | $R_{int} = 0.042$ |
| $T_{min} = 0.678$, $T_{max} = 0.803$ | $\theta_{max} = 30.0°$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0322P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | $+ 1.6142P]$ |
| $wR(F^2) = 0.073$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 5109 reflections | $\Delta\rho_{max} = 1.01$ e Å$^{-3}$ |
| 226 parameters | $\Delta\rho_{min} = -1.37$ e Å$^{-3}$ |
| H-atom parameters constrained | |

## Table 1
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ag—P | 2.3903 (4) | B—F2 | 1.372 (3) |
| Ag—F1 | 2.4242 (13) | B—F3 | 1.380 (2) |
| Ag—C3$^i$ | 2.5706 (18) | B—F1 | 1.411 (3) |
| B—F4 | 1.367 (3) | | |
| | | | |
| Ag···F3$^{ii}$ | 2.6912 (14) | Ag···F2 | 2.913 (2) |
| | | | |
| P—Ag—F1 | 148.19 (4) | F4—B—F1 | 109.54 (19) |
| P—Ag—C3$^i$ | 129.96 (5) | F2—B—F1 | 107.37 (18) |
| F1—Ag—C3$^i$ | 81.56 (6) | F3—B—F1 | 108.32 (17) |
| F4—B—F3 | 109.72 (17) | B—F1—Ag | 112.70 (12) |
| F2—B—F3 | 110.87 (19) | | |
| | | | |
| Ag—F1—B—F2 | −5.7 (2) | | |

Symmetry codes: (i) $-x + \frac{3}{2}$, $y - \frac{1}{2}$, $-z + \frac{1}{2}$; (ii) $-x + 1$, $-y$, $-z$.

H atoms were located in difference Fourier maps and placed in idealized positions, with C—H = 0.95 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The largest peak and deepest hole in the final difference map are located 0.75 and 0.60 Å from the Ag atom, respectively.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.
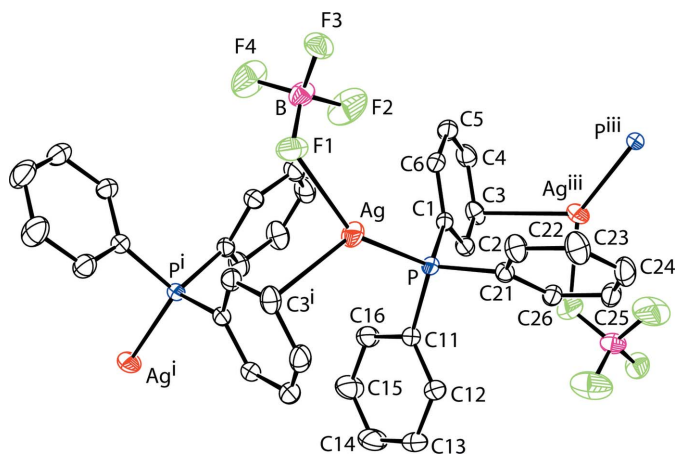


**Figure 1**
Part of the polymeric structure of (I), showing its polymeric nature. Displacement ellipsoids are shown at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $\frac{3}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$; (iii) $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$.]
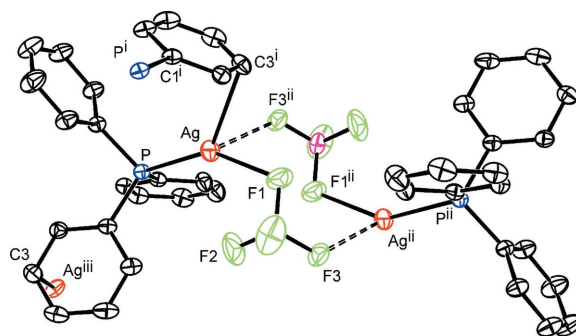


**Figure 2**
Two asymmetric units of (I), together with neighbouring Ag$^{iii}$ and C$_6$H$_5$P$^{ii}$ groups, showing the pairwise packing. Displacement ellipsoids are shown at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $\frac{3}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$; (ii) $1 - x$,-y,-z; (iii) $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$.]

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