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Tetrakis(triphenylphosphine)silver(I) tetraphenylborate acetonitrile solvate

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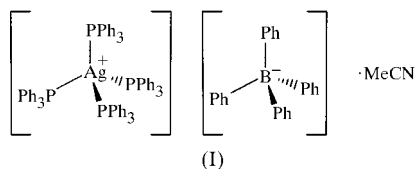
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In the title compound, $[\text{Ag}\{\text{P}(\text{C}_6\text{H}_5)\}_4][\text{B}\{\text{P}(\text{C}_6\text{H}_5)\}_4]\cdot\text{CH}_3\text{CN}$, the Ag ion resides on a crystallographic twofold rotation axis and is tetrahedrally coordinated. There is a disparity between the two independent Ag—P distances. This is due, in part, to the temperature differences (all previous determinations are at room temperature) but also to the packing effects of various anions.

Comment

In the title compound, (I), the Ag ion resides on a crystallographic twofold rotation axis and is tetrahedrally coordinated, with P—Ag—P angles ranging from 107.98 (7) to 111.02 (4)° [average 109.5 (13)°]. There is a disparity between the two independent Ag—P distances [2.6014 (13) and 2.6435 (14) Å], these values being somewhat shorter than those found in six related $[\text{Ag}\{\text{P}(\text{C}_6\text{H}_5)\}_4]^+$ cations in the Cambridge Structural Database (Version 5.18, April 2000; Allen & Kennard, 1993). This is, in part, due to the temperature differences (all previous determinations are at room temperature) but also the packing effects of various anions. The B atom in the tetraphenylborate anion and all the



non-H atoms in the acetonitrile solvent molecule are also located on twofold axes. The geometric parameters associated with the $[\text{BPh}_4]^-$ anion are normal. The solvent appears to be disordered across the twofold axis, resulting in a shorter than expected C—C bond. Complex (I) is isomorphous with an Au analogue also measured at 150 K (Jones, 1980), but shows none of the 7:1 tetrahedral—trigonal disorder associated with the central Au atom in the latter complex. The Ag—P distances are longer than the Au—P distances observed in

studies on isostructural Ag/Au phosphine complexes (Bowmaker *et al.*, 1997).

Experimental

The title compound was obtained while attempting to synthesize a silicate-based nitrogen pincer ligand coordinated to a platinum centre (Kleij *et al.*, 1999). The counter-ion in the synthesis was tetraphenylborate, whilst the triphenylphosphine was added to complete the coordination around the platinum. The complex decomposed in the presence of silver trifluoromethanesulfonate to give the final product. Colourless block-like crystals were obtained by recrystallization from a solution in acetonitrile. The colour changed to orange on irradiation in the X-ray beam.

Crystal data

$[\text{Ag}(\text{C}_{18}\text{H}_{15}\text{P})_4](\text{C}_{24}\text{H}_{20}\text{B})\cdot\text{C}_2\text{H}_3\text{N}$
 $M_r = 1517.21$
 Orthorhombic, *Ibca*
 $a = 21.763 (2) \text{ \AA}$
 $b = 22.955 (2) \text{ \AA}$
 $c = 30.767 (2) \text{ \AA}$
 $V = 15370 (2) \text{ \AA}^3$
 $Z = 8$
 $D_x = 1.311 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 Cell parameters from 22 reflections
 $\theta = 11.56\text{--}13.63^\circ$
 $\mu = 0.396 \text{ mm}^{-1}$
 $T = 150 (2) \text{ K}$
 Block, colourless
 $0.30 \times 0.30 \times 0.30 \text{ mm}$

Data collection

Enraf–Nonius CAD-4T diffractometer
 ω scans
 11 437 measured reflections
 6511 independent reflections
 3689 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.103$

$\theta_{\text{max}} = 25^\circ$
 $h = -5 \rightarrow 25$
 $k = -5 \rightarrow 27$
 $l = -36 \rightarrow 36$
 3 standard reflections
 frequency: 60 min
 intensity decay: 0.5%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.140$
 $S = 1.013$
 6511 reflections
 476 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0514P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.72 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ag1—P2	2.6014 (13)	Ag1—P1	2.6436 (14)
P2 ¹ —Ag1—P2	108.34 (6)	P2—Ag1—P1	109.24 (4)
P2 ¹ —Ag1—P1	111.02 (4)	P1 ¹ —Ag1—P1	107.98 (7)

Symmetry code: (i) $-x, \frac{1}{2} - y, z$.

The acetonitrile molecule is possibly disordered over the twofold axis resulting in large displacement parameters and a shorter than expected C—C bond. The orientation of the solvent was chosen with respect to that found in the isostructural Au complex (Jones, 1980). The R_{int} value is indicative of the large number of weak data. All H atoms were constrained (C—H = 0.95 and 0.98 Å) and allowed to ride on their C atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The methyl H atoms on the acetonitrile solvent are positionally disordered across the twofold axis.

Data collection: locally modified *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *DIRDIF* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *PLATON* (Spek, 2000).

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