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Bis(trimethylphosphine-κP)gold(I) hexafluorophosphate

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The title compound, $[\mathrm{Au(C_3H_9P)_2}]\mathrm{PF_6}$, a linear two-coordinate gold(I) complex with coordinated trimethylphosphine ligands and hexafluorophosphate as counter-ion, is isomorphous with $[\mathrm{Ag(Me_3P)_2}]\mathrm{PF_6}$ and exhibits similar bond distances to $[\mathrm{Au(Me_3P)_2}]\mathrm{Cl}$, thus unconditionally substantiating previous comparisons and claims that the ionic radius of Au is smaller than that of Ag. The cation has mirror symmetry, so that the P—Au—P axis lies in this plane. Similarly, the anion has mirror symmetry, with the plane containing an F—P—F axis.

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(P–F) = 0.004 Å
Disorder in main residue
R factor = 0.018
wR factor = 0.046
Data-to-parameter ratio = 18.8

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

Comment

In two separate recent publications, cationic bis(phosphine)complexes of Au and Ag have been compared in order to indicate the smaller ionic radius of $\mathrm{Au^I}$ relative to $\mathrm{Ag^I}$. Schmidbaur and co-workers (Bayler *et al.*, 1996) used trimesitylphosphine as a ligand in their comparative study, whereas Alyea *et al.* (2002) endeavoured to overcome the apparent intermolecular crowding and gold–mesityl methyl attractions in these complexes by comparing Ag—P bond distances in $[\mathrm{Ag(Me_3P)_2}]\mathrm{PF_6}$ with those in $[\mathrm{Au(Me_3P)_2}]\mathrm{Cl}$ (Angermaier *et al.*, 1994). The latter complex still maintains a weak [3.167 (1) Å] ion-pair contact.

$$[\mathrm{Me_3P} \longrightarrow \mathrm{Au} \longleftarrow \mathrm{PMe_3}]\,\mathrm{PF_6}$$

(I)

The unit cell of the title compound, $[\mathrm{Au(Me_3P)_2}]\mathrm{PF_6}$, (I), contains four formula units. The cation lies on a mirror plane, defined by atoms C2, P1, Au1, P2 and C3, as does the disordered $\mathrm{PF_6}^-$ anion, defined by atoms P3, F2 and F3. We have now crystallized (I) (Fig. 1 and Table 1), which is isomorphous with the Ag compound (Alyea *et al.*, 2002), and we report that the previous conclusions are substantiated by the fact that the distances and angles in $[\mathrm{Au(Me_3P)_2}]\mathrm{Cl}$ and $[\mathrm{Au(Me_3P)_2}]\mathrm{PF_6}$ are very similar: Au—P = 2.304 (1) and 2.3021 (9), and 2.3026 (9) Å, and P—Au—P = 175.4 (1) and 178.95 (3)°, respectively. Owing to disorder in the phosphine ligands of $[\mathrm{Au(Me_3P)_2}]\mathrm{Cl}$, the Au—P—C and C—P—C angles therein were not determined precisely enough to allow comparison. The corresponding angles in $[\mathrm{Au(Me_3P)_2}]\mathrm{PF_6}$ [113.14 (10)–114.62 (13) and 104.54 (13)–105.0 (12)°, respectively] are smaller and larger than the corresponding angles in the Ag compound $[\mathrm{Ag(Me_3P)_2}]\mathrm{PF_6}$ [114.0 (2)–114.9 (2) and 103.6 (2)–103.9 (2)°, respectively].

The closest Au$\cdots$F contact [Au1$\cdots$F6$^{\mathrm{i}}$ = 3.47 (2) Å; symmetry code: (i) $x, \frac{3}{2} - y, z$] is significantly longer than the distance reported for the corresponding Ag compound [3.392 (7) Å]. The very long Au···Au separation of 5.82 Å in (I) indicates that no intermolecular Au···Au interaction is present. The position of the PF_6^- anion relative to the complex in both the gold and silver complexes is similar.

Experimental

Compound (I) was formed during our attempts to prepare a cyclic gold(I) complex by reaction of deprotonated (BuLi) 1-methyl-3-prop-2-ynyl-3*H*-imidazolium hexafluorophosphate with chloro(trimethylphosphine)gold. The reaction product mixture was subsequently dissolved in dichloromethane, filtered over Celite to remove insoluble material and then layered with diethyl ether to form colourless crystals of (I) at room temperature.

Crystal data

$[Au(C_3H_9P)_2]PF_6$
$M_r = 494.08$
Orthorhombic, *Pnma*
$a = 11.4971$ (16) Å
$b = 8.5239$ (12) Å
$c = 14.317$ (2) Å
$V = 1403.1$ (3) Å^3
$Z = 4$
$D_x = 2.339$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 10.87$ mm^{-1}
$T = 100$ (2) K
Prism, colourless
0.20 × 0.15 × 0.13 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\min} = 0.161$, $T_{\max} = 0.243$
13950 measured reflections
1809 independent reflections
1766 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.046$
$S = 1.04$
1809 reflections
96 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 1.8242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.71$ e Å^{-3}
$\Delta\rho_{\min} = -0.66$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—P2	2.3021 (9)	P1—C2	1.811 (4)
Au1—P1	2.3026 (9)	P2—C4	1.806 (3)
P1—C1	1.804 (3)	P2—C3	1.809 (4)
P2—Au1—P1	178.95 (3)	C4^{i}—P2—C4	105.0 (2)
C1—P1—C1^{i}	105.8 (2)	C4—P2—C3	105.00 (12)
C1—P1—C2	104.54 (13)	C4—P2—Au1	113.14 (10)
C1—P1—Au1	113.70 (10)	C3—P2—Au1	114.62 (13)
C2—P1—Au1	113.65 (13)		

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

The complex crystallizes in the orthorhombic system, suggesting either the space group $Pn2_1a$ or *Pnma*, similar to its corresponding bis(trimethylphosphine)silver(I) hexafluorophosphate analogue (Alyea *et al.*, 2002). From solution and refinement, the space group *Pnma* was chosen. H atoms were included in the riding-model approximation, with C—H = 0.98 Å, and with $U_{\rm iso}(H) = 1.5 U_{\rm eq}(C)$. The site occupancies of the two sites in the disordered PF_6^- anion were refined to 0.865 (9):0.135 (9). The maximum residual electron-density peak of 1.71 e Å^{-3} is located 0.79 Å from the Au atom.

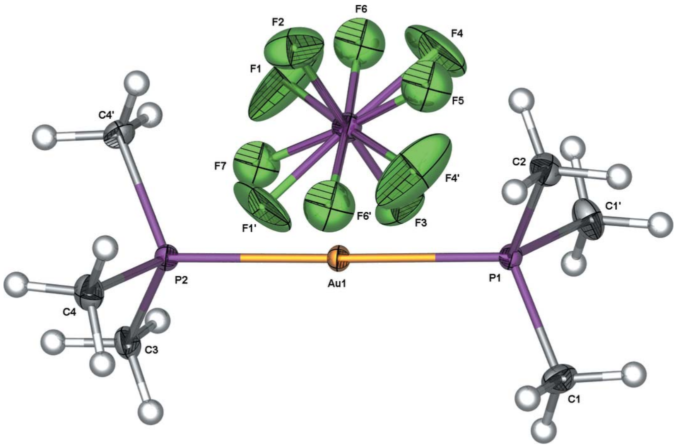

Figure 1
The molecular structure of (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level. Primed atoms are generated by the symmetry operator ($x, \frac{1}{2} - y, z$) in the caion and ($x, \frac{3}{2} - y, z$) in the anion.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Atwood & Barbour, 2003; Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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