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Chloro[tris(perfluorophenyl)phosphine]gold(I)

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The Au atom in the title compound, [AuCl{$(C_6F_5)_3P$}], exists within a P and Cl donor set that constitutes a linear geometry. There are two independent molecules in the asymmetric unit; the Au—P and Au—Cl bond lengths and the P—Au—Cl angle are 2.2060 (9), 2.2688 (9) Å and 172.68 (3)°, respectively, for molecule 1 and 2.2149 (9) 2.2706 (9) Å and 176.54 (3)°, respectively, for molecule 2.

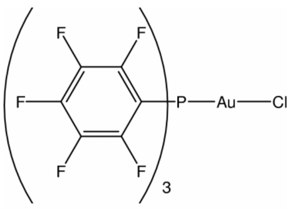
Key indicators

Single-crystal X-ray study
T = 183 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.074
Data-to-parameter ratio = 18.3

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

Comment

Phosphinegold(I) thiolates form an important class of compounds that display anti-arthritic activity and potential as antitumour agents (Tiekink, 2002). They are conveniently prepared from their phosphinegold(I) chloride precursors and it is in this context that the title compound, $(C_6F_5)_3PAuCl$, a known compound (Jacob *et al.*, 1997), was prepared and characterized. Two independent molecules comprise the asymmetric unit. The parameters defining the Au coordination geometry are in essential agreement with each other, and the Au—P distances are significantly shorter than the Au—Cl distances. The sequence of dihedral angles formed between the aromatic rings for molecule 1 are 76.89 (18), 73.83 (19) and 78.0 (2)°, and these values are closer than those found for molecule 2, *viz.* 65.73 (17), 68.74 (17) and 89.98 (18)°. As highlighted in Fig. 1, the two independent molecules are in close proximity so as to form weak Au...Cl interactions, such that Au1···Cl2 is 3.5428 (9) Å and Au2···Cl1 is shorter, at 3.4111 (9) Å. The Au1···Au2 separation is 3.7828 (3) Å. While there are many close F···F contacts in the crystal structure, the shortest contact involves atoms F15 and C3^{i} [symmetry code: (i) $-\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$]. A closer examination of this interaction reveals that, in fact, atom F15 is directed towards the ring centroid of the C1—C6 ring, so that this distance is 3.171 (3) Å, with an angle of 161.1 (3)° subtended at F15. A recent review emphasizes the importance of such interactions in the crystal structures of fluorinated molecules (Prasanna & Guru Row, 2000).



(I)

Experimental

The title compound was prepared from the reaction between $Na[AuCl_4]\cdot 2H_2O$ (Aldrich) and $(C_6F_5)_3P$ (Lancaster Synthesis) using established procedures (Al-Saády *et al.*, 1985). Colourless crystals were obtained in 72% yield from the layering of ethanol over a concentrated CH_2Cl_2 solution of the compound; m.p. 469.6 K (decomposition). Found: C 28.28%; $C_{18}AuClF_{15}P$ requires: C 28.36%. ^{13}C NMR ($CDCl_3$): δ 147.6 (*d, J* = 256 Hz), 145.2 (*d, J* = 258 Hz), 138.2 p.p.m. (*d, J* = 269 Hz) [P—C was not observed in accord with the literature (Jacob *et al.*, 1997)]. ^{19}F NMR ($CDCl_3$): δ −77.45 (*t*, 6F, *J* = 19 Hz), −90.57 (*d*, 3F, *J* = 23 Hz), −105.91 p.p.m. (*t*, 6F, *J* = 19 Hz). ^{31}P NMR ($CDCl_3$): δ −33.2 p.p.m.

Crystal data

$[AuCl(C_{18}F_{15}P)]$
M_r = 764.57
Monoclinic, $P2_1/n$
a = 15.4344 (7) Å
b = 11.8116 (5) Å
c = 22.4469 (10) Å
β = 95.632 (1)°
V = 4072.4 (3) Å^3
Z = 8
D_x = 2.494 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 8793 reflections
θ = 2.3–29.9°
μ = 7.58 mm^{-1}
T = 183 (2) K
Block, colourless
0.42 × 0.36 × 0.24 mm

Data collection

Bruker AXS SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.053, T_{max} = 0.162
33627 measured reflections
11871 independent reflections
8712 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 30.0°
$h = -20 \rightarrow 21$
$k = -13 \rightarrow 16$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
S = 1.01
11871 reflections
649 parameters
H atoms not located
$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.2060 (9)	P1—C7	1.824 (3)
Au1—Cl1	2.2688 (9)	P1—C13	1.814 (4)
Au2—P2	2.2149 (9)	P2—C19	1.820 (3)
Au2—Cl2	2.2706 (9)	P2—C25	1.820 (3)
P1—C1	1.813 (3)	P2—C31	1.805 (4)
P1—Au1—Cl1	172.68 (3)	C1—P1—C13	102.88 (16)
P2—Au2—Cl2	176.54 (3)	Au2—P2—C19	107.23 (11)
Au1—P1—C1	115.02 (11)	Au2—P2—C25	115.35 (11)
Au1—P1—C7	109.85 (11)	Au2—P2—C31	115.83 (12)
Au1—P1—C13	113.45 (12)	C19—P2—C25	107.31 (16)
C1—P1—C7	106.31 (15)	C19—P2—C31	109.03 (16)
C7—P1—C13	108.83 (16)	C25—P2—C31	101.68 (16)

The residual electron-density peak of 1.04 e Å^{-3} was located in the vicinity of the Au atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *PATTY* in *DIRDIF*92 (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXTL*.

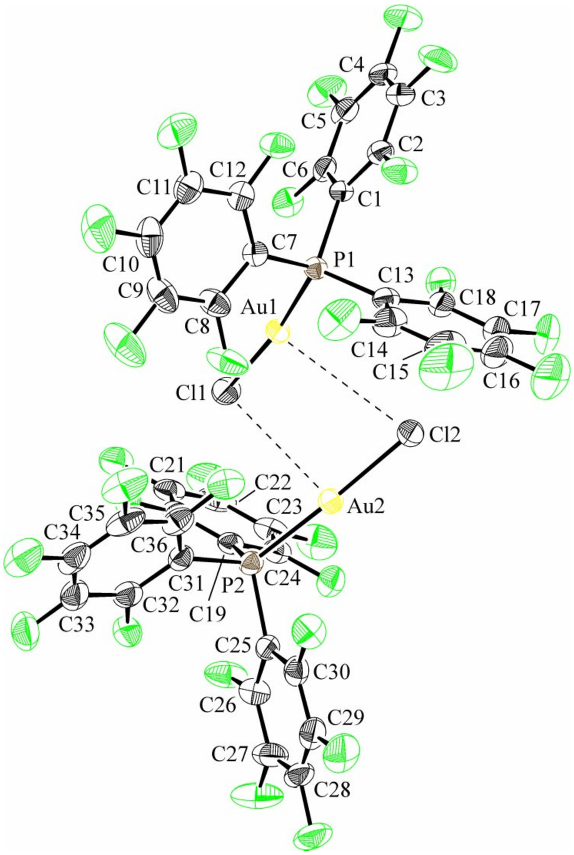


Figure 1
The molecular structure and crystallographic numbering scheme for the two independent molecules of $(C_6F_5)_3PAuCl$, highlighting the intermolecular Au···Cl contacts. Atom C20 is obscured. F atoms are labelled according to the atom to which they are bonded. Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

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