Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis[μ-bis(diphenylphosphino)methane]-digold(I) bis(hexafluorophosphate) dichloromethane disolvate

Meimei Wu, Liyi Zhang and Zhongning Chen*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: czn@ms.fjirsm.ac.cn

The dication in the title compound, $[Au_2(C_{25}H_{22}P_2)_2]$-$(PF_6)_2{\cdot}2CH_2Cl_2$ or $[Au_2(\mu\text{-dppm})_2](PF_6)_2{\cdot}2CH_2Cl_2$, where dppm is bis(diphenylphosphino)methane, is situated about a twofold axis and each anion lies on a mirror plane. Each Au atom is two-coordinate and exists in an approximately linear geometry.

Received 23 December 2002
Accepted 13 January 2003
Online 24 January 2003

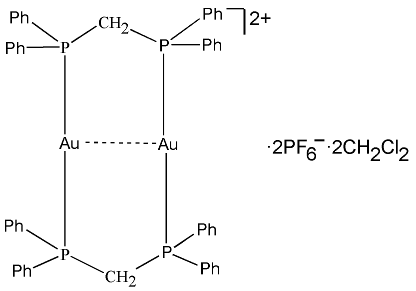
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.026 Å
R factor = 0.066
wR factor = 0.160
Data-to-parameter ratio = 14.5

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

Comment

Binuclear complexes of gold with certain bidentate ligands are of interest owing to their rich luminescence and bonding properties (Jaw *et al.*, 1989; Khan *et al.*, 1988; King *et al.*, 1989). In this context, several compounds of binuclear $[Au_2(\mu\text{-dppm})_2]^{2+}$ have been characterized previously (Jaw *et al.*, 1989; Khan *et al.*, 1989; Porter *et al.*, 1989; Liou *et al.*, 1994; Wang & Liu, 1994; Bauer & Schmidbaur, 1997), counterbalanced by various anionic species. Here we describe another crystal structure determination of the dication, in this case isolated as the hexafluorophosphate salt, $[Au_2(\mu\text{-dppm})_2](PF_6)_2{\cdot}2CH_2Cl_2$, (I) (Fig. 1 and Table 1).



(I)

The asymmetric unit of (I) comprises half a dication, $[Au_2(\mu\text{-dppm})_2]^{2+}$, situated about a twofold axis of symmetry, two independent PF_6^- anions, each lying on a mirror plane, and two molecules of dichloromethane. The Au atoms are doubly bridged by two dppm ligands. Each Au atom exists in the expected linear geometry, with the P1—Au—P2 angle being 177.85 (13)°. The intramolecular Au$\cdots$Au separation is 2.9792 (10) Å. The overall molecular geometry is in essential agreement with the previously determined structures cited above.

Experimental

The title compound was synthesized by a modification of a literature procedure (Porter *et al.*, 1989). The complex was obtained by the reaction between $[Au_2(\mu\text{-dppm})_2]Cl_2$ and $AgPF_6$ in a 1:2 ratio in acetonitrile solution under anaerobic conditions for 12 h. After the white precipitate, AgCl, was filtered off, the solution was evaporated under vacuum, affording $[Au_2(\mu\text{-dppm})_2](PF_6)_2$ in good yield. Wellformed colorless crystals suitable for X-ray diffraction measurements were grown by the slow diffusion of diethyl ether into a solution of the salt in a mixture of dichloromethane and a minimum of acetonitrile at room temperature.

Crystal data

$[Au_2(C_{25}H_{22}P_2)_2](PF_6)_2\cdot 2CH_2Cl_2$
$M_r = 1622.46$
Orthorhombic, *Pnma*
$a = 20.6825\ (10)$ Å
$b = 21.0325\ (9)$ Å
$c = 13.2577\ (6)$ Å
$V = 5767.2\ (5)$ Å^3
$Z = 4$
$D_x = 1.869$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 4469 reflections
$\theta = 1.8$–$25.1°$
$\mu = 5.51$ mm^{-1}
$T = 293\ (2)$ K
Block, colorless
0.42 × 0.40 × 0.20 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.121$, $T_{\max} = 0.332$
16736 measured reflections

5246 independent reflections
3249 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.097$
$\theta_{\max} = 25.1°$
$h = -24 \rightarrow 24$
$k = -20 \rightarrow 25$
$l = -15 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.160$
$S = 1.13$
5246 reflections
361 parameters
H-atom parameters constrained

$w = 1[\sigma^2(F_o^2) + (0.0355P)^2 + 11.5869P]$ where $P = (F_o^2 + 2F_c^2)3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.79$ e Å^{-3}
$\Delta\rho_{\min} = -1.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au—P1	2.314 (3)	P1—C21	1.804 (14)
Au—Au$^{\rm i}$	2.9792 (10)	P2—C2	1.821 (9)
P1—Au—P2	177.85 (13)	C1—P1—Au	111.1 (5)
P1—Au—Au$^{\rm i}$	91.18 (10)	C31—P2—C2	107.5 (8)
P2—Au—Au$^{\rm i}$	90.89 (9)	C31—P2—Au	114.0 (4)
C21—P1—C1	106.6 (8)	C41—P2—Au	113.1 (4)
C21—P1—Au	113.9 (5)	C2—P2—Au	110.7 (5)

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

The H atoms were positioned geometrically (C—H bonds lengths were fixed at 0.96 Å), assigned isotropic displacement parameters and allowed to ride on their respective parent C atoms. The maximum residual electron-density peak was located near the Au atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

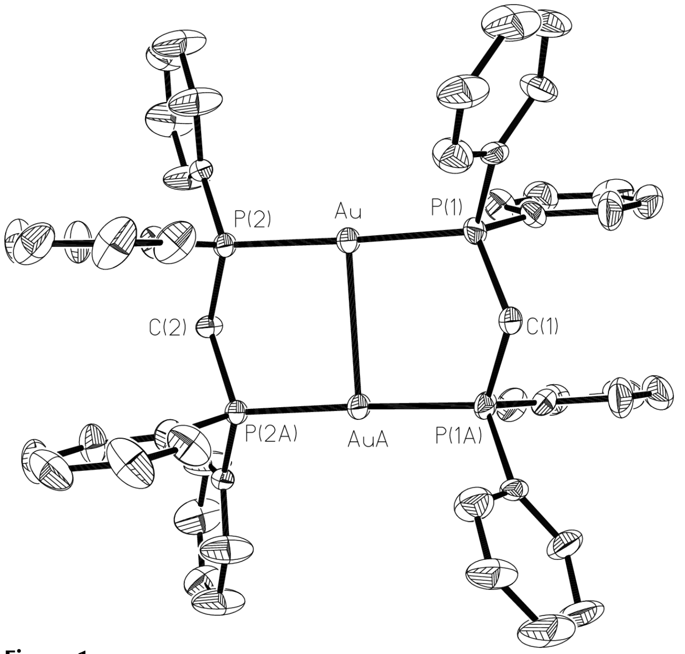


Figure 1
View of the dication of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

This work was supported by the NSF of China (No. 20171044).

References

Bauer, A. & Schmidbaur, H. (1997). *J. Chem. Soc. Dalton Trans.* pp. 1115–1116.
Jaw, H. R. C., Savas, M. M., Rogers, R. D. & Mason, W. R. (1989). *Inorg. Chem.* **29**, 1028–1037.
Khan, M. N. I., Fackler, J. P. Jr, King, C., Wang, J. C. & Wang, S. (1988). *Inorg. Chem.* **28**, 1672–1673.
Khan, M. N. I., King, C., Heinrich, D. D., Fackler, J. P. Jr & Porter, L. C. (1989). *Inorg. Chem.* **29**, 2150–2154.
King, C., Wang, J. C., Khan, M. N. I. & Fackler, J. P. Jr (1989). *Inorg. Chem.* **29**, 2145–2149.
Liou, L. S., Liu, C. P. & Wang, J. C. (1994). *Acta Cryst.* C**50**, 538–540.
Porter, L. C., Khan, M. N. I., King, C. & Fackler, J. P. Jr (1989). *Acta Cryst.* C**45**, 947–949.
Sheldrick, G.. (1996). *SADABS*. University of Göttingen, Germany.
Siemens (1994). *SAINT* and *SHELXTL Reference Manuals*. Version 5. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART Reference Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, J. C. & Liu. L. K. (1994). *Acta Cryst.* C**50**, 704–706.