Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bromo[(diphenylphosphino-κ*P*)(diphenylphosphinoyl)methane]gold(I) acetonitrile solvate

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Received 1 August 2003
Accepted 11 August 2003
Online 23 August 2003

In the title compound, [AuBr(dppmO)]·CH_3CN [dppmO = $Ph_2P(CH_2)P(O)Ph_2$], the dppmO ligand coordinates through the P donor to give a linear two-coordinate P—Au—Br gold(I) complex. The Au—Br and Au—P bond lengths are 2.241 (2) and 2.4069 (19) Å, respectively. The P—Au—Br and P═O groups lie almost parallel to each other [O—P···P—Au = 8.3 (2)°], while the intramolecular Au···O distance is 3.274 (4) Å.

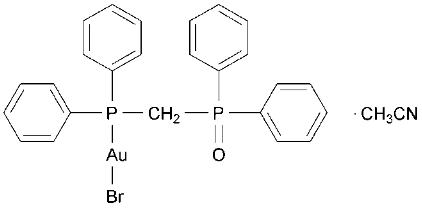
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.030
wR factor = 0.079
Data-to-parameter ratio = 20.2

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

Comment

Mixed bidentate phosphine–phosphine oxide ligands of general formula $R_2P—Y—P(O)R_2$, where Y is an organic spacer group, represent an important class of bidentate chelating ligands incorporating both soft (P) and hard (O) donor atoms (Grushin, 2001). Transition metal complexes of these ligands show a variety of structural forms (*e.g.* Coyle *et al.*, 1998; Saravanabharathi *et al.*, 2002; Faller & Parr, 2000) with evidence for both bidentate and monodentate coordination of the ligand to the metal atom.



(I)

We report here the structure of the acetonitrile solvate of the 1:1 complex of $Ph_2P(CH_2)P(O)Ph_2$ with gold(I) bromide, [(dppmO)AuBr]·CH_3CN, (I). The structure comprises discrete molecules of [(dppmO)AuBr] and acetonitrile separated by normal van der Waals distances (Fig. 1). The dppmO ligand coordinates to the gold through the P atom to yield a linear two-coordinate P—Au—Br geometry, with Au—P = 2.241 (2) Å, Au—Br = 2.4069 (19) Å and P—Au—Br = 178.53 (4)°. These parameters are similar to those recorded for other two-coordinate R_3PAuBr complexes (Bott *et al.*, 2000). The P═O bond length of 1.490 (3) Å is also in accord with values recorded for other phosphine oxides (See *et al.*, 1998).

The P—Au—Br and P═O groups lie almost parallel, with the torsion angle O—P···P—Au 8.3 (2)°. For comparison, in the structure of the benzene solvate of the dioxide, $dppmO_2$ (Antipin *et al.*, 1980), the P═O bonds are almost antiparallel, whereas in the structures of adducts of $dppmO_2$ with sodium halides (Hewertson *et al.*, 1970; Ding *et al.*, 2000) coordination of the O atoms to the sodium cation results in parallel P═O bonds and an Na···O distance of 2.457 (1) Å. An intermediate situation is observed for the structure of the 2:1 gold chloride complex with dppm, $[(AuCl)_2(dppm)]$ (Schmidbaur *et al.*, 1977), where the Au—P···P—Au torsion angle is 67 (1)°, with an Au···Au distance of 3.351 (2) Å, the latter suggestive of significant aurophilic interaction. In the present complex, the intramolecular Au···O distance of 3.274 (4) Å is slightly longer than the Au···O distances for the [(tmpp)Au*X*] complexes [*X* = Cl, Br, I; tmpp = tris(2,4,6-trimethoxyphenyl)phosphine)] (Baker *et al.*, 1995), which are in the range 2.92 (2)–3.15 (1) Å. This result, together with the absence of any significant distortion from linearity of the P—Au—Br bond, indicates the presence of only weak, if any, bonding interactions between the Au and O atoms and that the conformational structure of the complex is best ascribed as an outcome of crystal-packing considerations.

Experimental

$[NBu_4][AuBr_2]$ (50 mg, 0.083 mmol) and diphenylphosphinomethane mono-oxide (dppmO, 33.4 mg, 0.083 mmol) were dissolved in acetonitrile (10 ml) to give a clear solution. Slow evaporation of the solvent yielded well formed, colorless crystals of (I); m.p. 506–507 K. The crystals slowly lost solvent over a period of weeks. Analysis found: C 46.0, H 3.5 N 1.7%; calculated for $C_{27}H_{25}AuBrNOP_2$: C 45.15, H 3.51, N 1.95%.ν_{max} (KBr)/cm^{-1}: 1179 (P=O str). δ_H (400 MHz, $CDCl_3$, p.p.m.): 3.53 [2H, *dd*, CH_2, $^2J_{P(Au)CH}$ = 12 Hz, $^2J_{P(O)CH}$ = 12 Hz], 7.36–7.47 (8H, *m*, *m*-C_6H_5), 7.42–7.55 (4H, *m*, *p*-C_6H_5), 7.66–7.75 (8H, *m*, *o*-C_6H_5). δ_C (100 MHz, $CDCl_3$, p.p.m.): 31.4 [*dd*, CH_2, $^1J_{CP(O)}$ = 59 Hz, $^1J_{CP(Au)}$ = 26 Hz], 129.4 [*d*, *m*-C_6H_5(PAu), $^3J_{CP(Au)}$ = 12 Hz], 129.4 [*d*, *m*-C_6H_5(PO), $^3J_{CP(O)}$ = 12 Hz], 129.7 [*dd*, *i*-C_6H_5(PAu), $^1J_{CP(Au)}$ = 61 Hz, $^3J_{CP(O)}$ = 4 Hz], 131.2 [*d*, *o*-C_6H_5(PAu), $^2J_{CP(Au)}$ = 10 Hz], 131.9 [*dd*, *i*-C_6H_5(PO), $^1J_{CP(O)}$ = 105 Hz, $^3J_{CP(Au)}$ = 3 Hz], 132.3 [*d*, *p*-C_6H_5(PAu), $^4J_{CP(Au)}$ = 3 Hz], 132.9 [*d*, *p*-C_6H_5(PO), $^4J_{CP(O)}$ = 3 Hz], 133.7 [*d*, *o*-C_6H_5(PO), $^2J_{CP(O)}$ = 15 Hz], δ_P (162 MHz, $CDCl_3$, p.p.m.): 25.0 [*s*, P(O)]; 20.0 [*s*, P(Au)].

Crystal data

$[AuBr(C_{25}H_{22}OP_2)]\cdot CH_3CN$
$M_r = 718.29$
Monoclinic, $P2_1/c$
$a = 11.657\ (3)$ Å
$b = 22.436\ (17)$ Å
$c = 11.209\ (4)$ Å
$\beta = 115.98\ (2)^\circ$
$V = 2635\ (2)$ Å^3
$Z = 4$

$D_x = 1.811$ Mg m^{-3}
Mo Kα radiation
Cell parameters from 25 reflections
$\theta = 12.5–17.4^\circ$
$\mu = 7.24$ mm^{-1}
$T = 295$ K
Prism, colorless
0.30 × 0.30 × 0.20 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.135$, $T_{max} = 0.235$
6598 measured reflections
6045 independent reflections
4561 reflections with $I > 2\sigma(I)$

$R_{int} = 0.027$
$\theta_{max} = 27.5^\circ$
$h = -13 \rightarrow 15$
$k = 0 \rightarrow 29$
$l = -14 \rightarrow 5$
3 standard reflections every 150 reflections
intensity decay: 5.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.02$
6045 reflections
299 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 2.0179P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -1.07$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00103 (10)

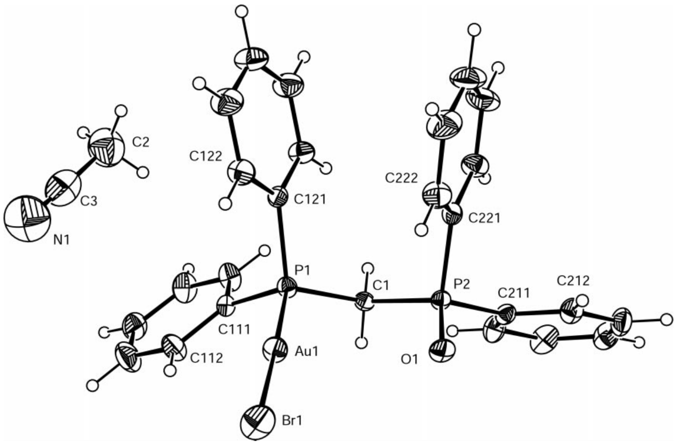


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

Au1—Br1	2.4069 (19)	P2—O1	1.490 (3)
Au1—P1	2.241 (2)	P2—C1	1.812 (5)
P1—C1	1.825 (5)	P2—C211	1.807 (5)
P1—C111	1.820 (5)	P2—C221	1.804 (5)
P1—C121	1.822 (5)	N1—C3	1.105 (14)
Br1—Au1—P1	178.53 (4)	C211—P2—C221	105.8 (2)
Au1—P1—C1	114.21 (15)	P1—C1—P2	115.0 (2)
Au1—P1—C111	113.87 (14)	P1—C111—C112	120.0 (4)
Au1—P1—C121	113.16 (14)	P1—C111—C116	121.0 (4)
C1—P1—C111	103.0 (2)	P1—C121—C126	122.7 (3)
C1—P1—C121	108.1 (2)	P1—C121—C122	117.7 (3)
C111—P1—C121	103.5 (2)	N1—C3—C2	177.9 (11)
O1—P2—C1	113.2 (2)	P2—C211—C216	125.1 (4)
O1—P2—C211	112.7 (2)	P2—C211—C212	115.7 (3)
O1—P2—C221	112.0 (2)	P2—C221—C222	118.8 (4)
C1—P2—C211	106.2 (2)	P2—C221—C226	121.5 (4)
C1—P2—C221	106.4 (2)		

H atoms were constrained in the riding model approximation, fixed to their parent C atoms at a C—H distance of 0.95 Å, and U_{iso}(H) values were set to $1.2U_{eq}$ of the parent atom. The maximum and minimum residual electron density peaks were located within 1 Å of atom Au1.

Data collection: *MSC/AFC-7 Diffractometer Control Software for Windows* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software for Windows*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: *TEXSAN for Windows*; program(s) used to refine structure: *TEXSAN for Windows* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *TEXSAN for Windows* and *PLATON* (Spek, 1980–2001).

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Acta Cryst. (2003). E**59**, m768–m770 Michael L. Williams *et al.* • $[AuBr(C_{25}H_{22}OP_2)]\cdot CH_3CN$ **m769**

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