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Bis[2-(diphenylphosphanyl-κP)-benzaldehyde]iodidogold(I)

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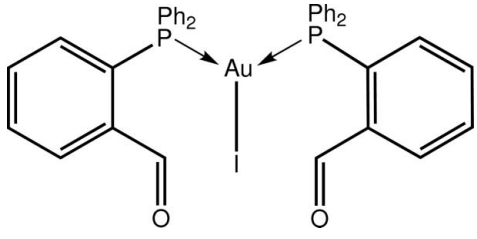
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.059; data-to-parameter ratio = 24.0.

In the title compound, $[AuI(C_{19}H_{15}OP)_2]$, the complete molecule is generated by the application of twofold symmetry. The Au^I atom is in a trigonal–planar geometry within an IP_2 donor set with the greatest distortion seen in the P—Au—P angle [128.49 (3) °]. Close intramolecular Au···O interactions [3.172 (3) Å] are observed. No specific intermolecular interactions are noted in the crystal packing.

Related literature

For a discussion on intramolecular Au···O interactions, see: Kuan *et al.* (2008). For related structures, see: Bowmaker *et al.* (1987); Elsegood *et al.* (2006).



Experimental

Crystal data

$[AuI(C_{19}H_{15}OP)_2]$
M_r = 904.43
Monoclinic, $C2/c$
a = 18.1099 (13) Å
b = 10.1856 (6) Å
c = 19.8438 (13) Å
β = 115.965 (2)°
V = 3290.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.54 mm^{-1}
T = 223 K
0.40 × 0.30 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.392, T_{max} = 1.000
13430 measured reflections
4792 independent reflections
4319 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.059
S = 1.01
4792 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −1.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au—I1	2.7188 (3)	Au—P1	2.3200 (6)
P1—Au—I1	115.755 (16)	P1^{i}—Au—P1	128.49 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2394).

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supplementary materials

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Bis[2-(diphenylphosphanyl-κP)benzaldehyde]iodidogold(I)

Michael L. Williams, Samuel P. C. Dunstan, Peter C. Healy and Edward R. T. Tiekink

Comment

The crystal structure of the monophosphinegold(I) chloride complex, (2-$CHOC_6H_4$)Ph_2PAuCl, where one of the organic substituents on the phosphine has been functionalized with an aldehyde group, has been reported previously (Elsegood *et al.*, 2006). Herein, the crystal structure of the title bis(phosphine)gold(I) iodide analogue (I) is described.

In (I), Fig. 1, the complete molecule is generated by the application of twofold symmetry. The Au atom is in a trigonal planar geometry within a IP_2 donor set, Table 1, with the greatest distortion manifested in the angle, *i.e.* 128.49 (3)°, subtended by the phosphine ligands, Table 1. The Au—I and Au—P bond lengths in the comparable $(Ph_3P)_2AuI$ complex, which also has crystallographic twofold symmetry are 2.754 (1) and 2.333 (2) Å, respectively (Bowmaker *et al.*, 1987); the P—Au—P angle is 132.13 (7)°.

In (I), close intramolecular Au···O interactions of 3.172 (3) Å are noted. Similar interactions of 3.109 (4) and 3.106 (4) Å (two independent molecules) were observed in (2-$CHOC_6H_4$)Ph_2PAuCl (Elsegood *et al.*, 2006) and their significance has been discussed in the literature (Kuan *et al.*, 2008).

No specific intermolecular interactions are noted in the crystal packing. Globally, molecules are arranged in layers that stack along the *c* axis.

Experimental

$[NBu_4][AuI_2]$ (100 mg, 0.184 mmol) and (2-$CHOC_6H_4$)Ph_2P (107 mg, 0.368 mmol) were dissolved in warm DMF (10 ml) to give a clear solution. Cooling to room temperature and slow evaporation of solvent yielded clear, colourless crystals of the title complex. *M*.pt: 471–283 K. Analysis: Found C 50.33, H 3.34%. Calculated for $C_{38}H_{30}AuIO_2P_2$: C 50.46, H 3.34%.

Refinement

The H atoms were geometrically placed (C—H = 0.94–0.99 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum and minimum residual electron density peaks of 1.47 and 1.34 e $Å^{-3}$, respectively, were located 0.82 Å and 0.86 Å from the Au atom.

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

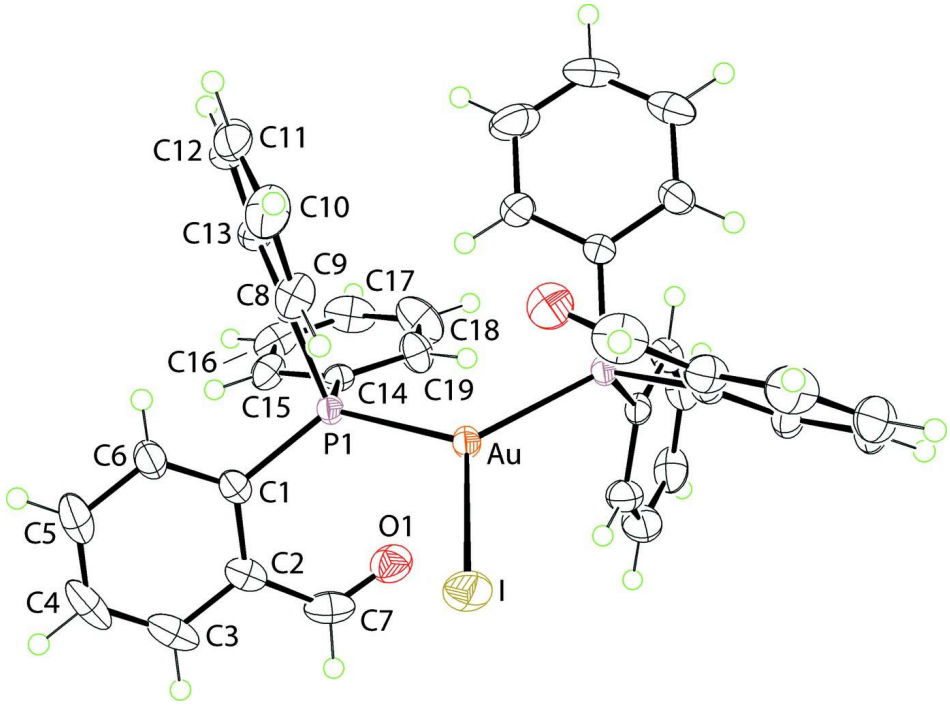

Figure 1

Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level. The molecule has twofold symmetry and unlabelled atoms are related by the symmetry operation 2 - *x*, *y*, 1/2 - *z*.

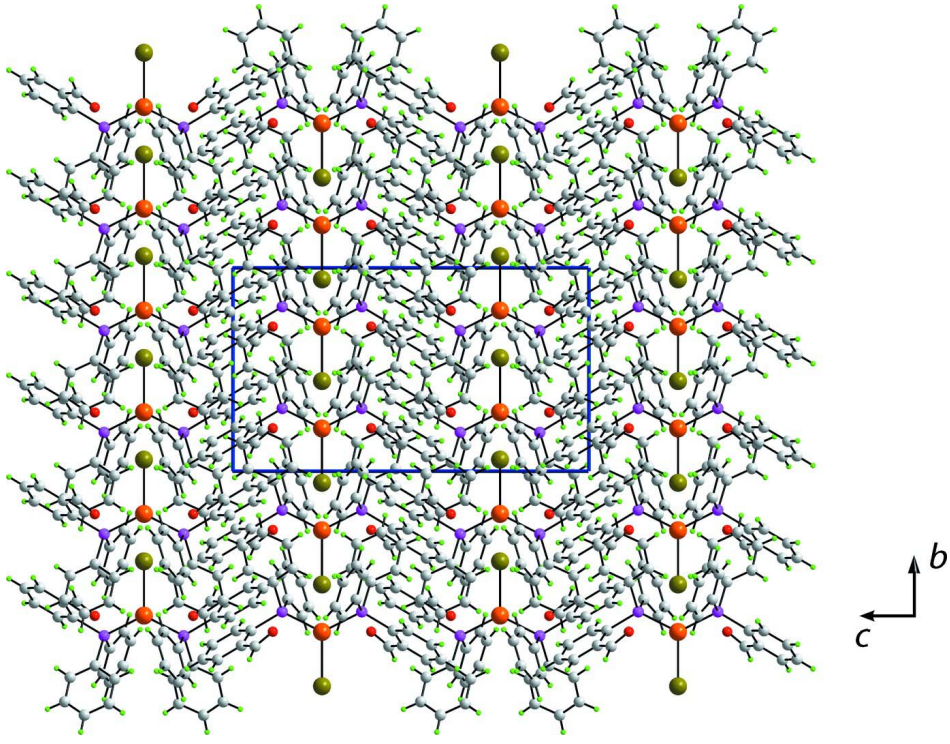

Figure 2

A view in projection down the *a* axis of the unit-cell contents of (I).

Bis[2-(diphenylphosphanyl-κ*P*)benzaldehyde]iodidogold(I)

Crystal data

$[AuI(C_{19}H_{15}OP)_2]$
$M_r = 904.43$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 18.1099$ (13) Å
$b = 10.1856$ (6) Å
$c = 19.8438$ (13) Å
$\beta = 115.965$ (2)°
$V = 3290.9$ (4) Å^3
$Z = 4$
$F(000) = 1744$
$D_x = 1.825$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 7249 reflections
$\theta = 2.1$–$40.5°$
$\mu = 5.54$ mm^{-1}
$T = 223$ K
Prism, colourless
0.40 × 0.30 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.392$, $T_{max} = 1.000$
13430 measured reflections
4792 independent reflections
4319 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.3°$
$h = -25 \rightarrow 25$
$k = -9 \rightarrow 14$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.059$
$S = 1.01$
4792 reflections
200 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.47$ e Å^{-3}
$\Delta\rho_{min} = -1.34$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au	1.0000	0.290105 (13)	0.2500	0.02140 (5)
I1	1.0000	0.55703 (3)	0.2500	0.04282 (8)
P1	1.01880 (4)	0.19113 (6)	0.36168 (3)	0.01989 (13)
O1	1.17648 (14)	0.2889 (2)	0.38822 (14)	0.0404 (5)
C1	1.05497 (18)	0.2836 (2)	0.44986 (15)	0.0245 (5)

C2	1.12816 (18)	0.3569 (3)	0.47629 (17)	0.0329 (6)
C3	1.1539 (2)	0.4272 (3)	0.5433 (2)	0.0478 (9)
H3	1.2025	0.4768	0.5609	0.057*
C4	1.1084 (3)	0.4246 (3)	0.58394 (19)	0.0512 (10)
H4	1.1263	0.4716	0.6291	0.061*
C5	1.0371 (2)	0.3533 (3)	0.55821 (16)	0.0430 (8)
H5	1.0064	0.3510	0.5860	0.052*
C6	1.0100 (2)	0.2843 (3)	0.49109 (16)	0.0327 (7)
H6	0.9604	0.2373	0.4735	0.039*
C7	1.1813 (2)	0.3609 (4)	0.4379 (2)	0.0453 (8)
H7	1.2227	0.4252	0.4535	0.054*
C8	0.91749 (15)	0.1302 (3)	0.34615 (13)	0.0218 (5)
C9	0.8497 (2)	0.2101 (3)	0.30578 (18)	0.0345 (7)
H9	0.8577	0.2944	0.2908	0.041*
C10	0.7712 (2)	0.1663 (4)	0.28772 (19)	0.0447 (8)
H10	0.7262	0.2214	0.2605	0.054*
C11	0.7575 (2)	0.0440 (4)	0.30874 (18)	0.0414 (8)
H11	0.7038	0.0160	0.2970	0.050*
C12	0.8231 (2)	−0.0368 (3)	0.34700 (17)	0.0368 (7)
H12	0.8142	−0.1213	0.3610	0.044*
C13	0.90263 (17)	0.0048 (3)	0.36533 (15)	0.0287 (6)
H13	0.9469	−0.0524	0.3910	0.034*
C14	1.08135 (16)	0.0436 (2)	0.38691 (14)	0.0212 (5)
C15	1.10862 (17)	−0.0130 (3)	0.45739 (16)	0.0307 (6)
H15	1.1002	0.0308	0.4951	0.037*
C16	1.14815 (18)	−0.1334 (3)	0.47260 (19)	0.0391 (7)
H16	1.1675	−0.1700	0.5208	0.047*
C17	1.1591 (2)	−0.1991 (3)	0.4175 (2)	0.0447 (9)
H17	1.1839	−0.2824	0.4274	0.054*
C18	1.1339 (2)	−0.1434 (4)	0.3476 (2)	0.0519 (9)
H18	1.1424	−0.1880	0.3101	0.062*
C19	1.09597 (19)	−0.0217 (3)	0.33260 (16)	0.0334 (6)
H19	1.0800	0.0170	0.2853	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au	0.02340 (8)	0.02290 (8)	0.01865 (7)	0.000	0.00992 (5)	0.000
I1	0.0565 (2)	0.02093 (14)	0.0547 (2)	0.000	0.02773 (17)	0.000
P1	0.0234 (3)	0.0198 (3)	0.0171 (3)	0.0003 (2)	0.0095 (3)	0.0002 (2)
O1	0.0317 (12)	0.0451 (14)	0.0453 (14)	−0.0044 (10)	0.0176 (10)	−0.0003 (11)
C1	0.0315 (14)	0.0184 (13)	0.0201 (12)	0.0036 (10)	0.0081 (11)	0.0012 (10)
C2	0.0316 (16)	0.0266 (15)	0.0329 (15)	−0.0010 (12)	0.0070 (12)	−0.0041 (12)
C3	0.048 (2)	0.0341 (18)	0.043 (2)	−0.0060 (15)	0.0031 (17)	−0.0143 (14)
C4	0.070 (3)	0.0409 (19)	0.0264 (17)	0.0090 (17)	0.0058 (17)	−0.0148 (14)
C5	0.065 (2)	0.0395 (19)	0.0250 (15)	0.0110 (17)	0.0197 (15)	−0.0016 (13)
C6	0.0443 (18)	0.0297 (16)	0.0256 (14)	−0.0004 (12)	0.0167 (13)	−0.0037 (11)
C7	0.0307 (17)	0.0416 (19)	0.055 (2)	−0.0137 (15)	0.0108 (15)	−0.0047 (17)
C8	0.0232 (13)	0.0254 (13)	0.0177 (11)	−0.0004 (11)	0.0097 (10)	−0.0018 (10)
C9	0.0330 (16)	0.0359 (17)	0.0383 (16)	0.0090 (13)	0.0189 (14)	0.0083 (13)

C10	0.0277 (16)	0.064 (2)	0.0415 (19)	0.0130 (16)	0.0147 (15)	0.0103 (17)
C11	0.0278 (16)	0.065 (2)	0.0333 (17)	−0.0088 (15)	0.0149 (14)	−0.0056 (15)
C12	0.0380 (18)	0.0402 (17)	0.0342 (16)	−0.0158 (14)	0.0177 (14)	−0.0038 (13)
C13	0.0285 (14)	0.0298 (15)	0.0263 (13)	−0.0023 (12)	0.0106 (11)	0.0024 (11)
C14	0.0188 (12)	0.0208 (12)	0.0225 (12)	−0.0012 (10)	0.0075 (10)	0.0006 (10)
C15	0.0258 (14)	0.0359 (16)	0.0305 (14)	0.0028 (12)	0.0124 (12)	0.0083 (12)
C16	0.0251 (15)	0.0381 (17)	0.0478 (19)	0.0041 (13)	0.0102 (14)	0.0174 (15)
C17	0.0318 (17)	0.0269 (17)	0.059 (2)	0.0096 (13)	0.0052 (16)	0.0034 (15)
C18	0.052 (2)	0.042 (2)	0.053 (2)	0.0166 (17)	0.0151 (18)	−0.0146 (17)
C19	0.0378 (17)	0.0335 (16)	0.0276 (14)	0.0088 (13)	0.0130 (13)	−0.0011 (12)

Geometric parameters (Å, º)

Au—P1^{i}	2.3200 (6)	C9—C10	1.381 (4)
Au—I1	2.7188 (3)	C9—H9	0.9400
Au—P1	2.3200 (6)	C10—C11	1.370 (5)
P1—C14	1.816 (3)	C10—H10	0.9400
P1—C1	1.837 (3)	C11—C12	1.369 (5)
P1—C8	1.831 (3)	C11—H11	0.9400
O1—C7	1.200 (4)	C12—C13	1.388 (4)
C1—C6	1.384 (4)	C12—H12	0.9400
C1—C2	1.407 (4)	C13—H13	0.9400
C2—C3	1.398 (4)	C14—C15	1.388 (4)
C2—C7	1.467 (5)	C14—C19	1.387 (4)
C3—C4	1.383 (6)	C15—C16	1.385 (4)
C3—H3	0.9400	C15—H15	0.9400
C4—C5	1.369 (5)	C16—C17	1.368 (5)
C4—H4	0.9400	C16—H16	0.9400
C5—C6	1.392 (4)	C17—C18	1.378 (5)
C5—H5	0.9400	C17—H17	0.9400
C6—H6	0.9400	C18—C19	1.384 (4)
C7—H7	0.9400	C18—H18	0.9400
C8—C9	1.396 (4)	C19—H19	0.9400
C8—C13	1.392 (4)		
P1—Au—I1	115.755 (16)	C10—C9—C8	120.5 (3)
P1^{i}—Au—P1	128.49 (3)	C10—C9—H9	119.8
P1^{i}—Au—I1	115.755 (16)	C8—C9—H9	119.8
C14—P1—C1	104.04 (12)	C9—C10—C11	121.2 (3)
C14—P1—C8	102.94 (12)	C9—C10—H10	119.4
C1—P1—C8	104.32 (12)	C11—C10—H10	119.4
C14—P1—Au	115.85 (9)	C12—C11—C10	119.1 (3)
C1—P1—Au	121.94 (8)	C12—C11—H11	120.4
C8—P1—Au	105.63 (8)	C10—C11—H11	120.4
C6—C1—C2	118.6 (3)	C11—C12—C13	120.7 (3)
C6—C1—P1	120.6 (2)	C11—C12—H12	119.6
C2—C1—P1	120.8 (2)	C13—C12—H12	119.6
C3—C2—C1	119.5 (3)	C12—C13—C8	120.7 (3)
C3—C2—C7	117.3 (3)	C12—C13—H13	119.7
C1—C2—C7	123.1 (3)	C8—C13—H13	119.7

C4—C3—C2	120.6 (3)	C15—C14—C19	118.6 (3)
C4—C3—H3	119.7	C15—C14—P1	121.7 (2)
C2—C3—H3	119.7	C19—C14—P1	119.4 (2)
C5—C4—C3	119.8 (3)	C14—C15—C16	120.6 (3)
C5—C4—H4	120.1	C14—C15—H15	119.7
C3—C4—H4	120.1	C16—C15—H15	119.7
C4—C5—C6	120.3 (3)	C17—C16—C15	120.0 (3)
C4—C5—H5	119.8	C17—C16—H16	120.0
C6—C5—H5	119.8	C15—C16—H16	120.0
C5—C6—C1	121.1 (3)	C16—C17—C18	120.2 (3)
C5—C6—H6	119.5	C16—C17—H17	119.9
C1—C6—H6	119.5	C18—C17—H17	119.9
O1—C7—C2	125.5 (3)	C19—C18—C17	120.0 (3)
O1—C7—H7	117.2	C19—C18—H18	120.0
C2—C7—H7	117.2	C17—C18—H18	120.0
C9—C8—C13	117.7 (2)	C18—C19—C14	120.5 (3)
C9—C8—P1	117.6 (2)	C18—C19—H19	119.8
C13—C8—P1	124.4 (2)	C14—C19—H19	119.8

Symmetry code: (i) $-x+2$, y, $-z+1/2$.