

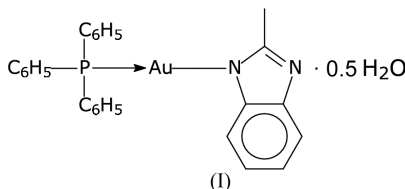
(2-Methylbenzimidazolyl- κN)(triphenylphosphine- κP)gold(I) hemihydrateDan Li,^{a*} Tao Wu^a and
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.012$ Å
 R factor = 0.038
 wR factor = 0.092
Data-to-parameter ratio = 16.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The Au^I atom in the title compound, [Au(C₈H₇N₂)(C₁₈H₁₅P)]·0.5H₂O, shows a linear coordination. The tertiary N atom of the anionic group interacts with the uncoordinated water molecule, which lies on a twofold axis.

Comment

An earlier study provided details of the crystal structure of the 1/1 benzimidazolylgold(I) adduct with triphenylphosphine, whose metal atom shows linear coordination [Au—N = 2.022 (5) Å and Au—P = 2.232 (2) Å; N—Au—P = 179.6 (1)°] (Li *et al.*, 2004). In the title compound, (I), the introduction of a methyl substituent in the anion leads to only minor changes in the bond dimensions of the Au^I atom, as shown in Fig. 1 and Table 1. The 180° angle in the unsubstituted adduct is reduced to 175.3 (2)° in the methyl-substituted adduct; the decrease can be attributed to the steric bulk of the methyl group. The non-coordinated atom N2 engages in hydrogen bonding with the uncoordinated water molecule, forming a hydrogen-bonded assembly of two complexes and one water molecule (Table 2).

Experimental

To a solution of chloro(triphenylphosphine)gold (0.99 g, 2.0 mmol) and 2-methylbenzimidazole (0.27 g, 2.0 mmol) in acetone (20 ml) was added 1 M sodium hydroxide (2 ml). The solution was stirred for 2 h; the precipitated sodium chloride was removed and the filtrate concentrated to give a colorless compound that was recrystallized from dichloromethane (10 ml). Prismatic crystals were obtained by diffusing diethyl ether into a dichloromethane solution of the compound; the yield was about 75%. CHN elemental analysis calculated for C₂₆H₂₃AuN₂O_{0.5}P: C 52.09, H 3.76, N 4.67%; found: C 52.10, H 3.87, N 4.67%. IR (KBr)/cm⁻¹: 3424 (*m*), 3052 (*w*), 2914 (*m*), 1607 (*m*), 1483 (*m*), 1436 (*s*), 1350 (*m*), 1226 (*s*), 1106 (*s*), 999 (*m*), 759 (*s*), 742 (*s*), 699 (*s*), 540 (*s*), 510 (*m*).

Crystal data

[Au(C₈H₇N₂)(C₁₈H₁₅P)]·0.5H₂O
 $M_r = 599.40$
 Orthorhombic, *Pbcn*
 $a = 26.2518$ (9) Å
 $b = 9.3899$ (4) Å
 $c = 18.4960$ (6) Å
 $V = 4559.3$ (3) Å³
 $Z = 8$
 $D_x = 1.746$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 4375 reflections
 $\theta = 2.6$ – 25.1°
 $\mu = 6.54$ mm⁻¹
 $T = 293$ (2) K
 Block, colorless
 $0.40 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART area-detector
diffractometer
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 1999)
 $T_{\min} = 0.137$, $T_{\max} = 0.270$
10 540 measured reflections

4010 independent reflections
2733 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 25.1^\circ$
 $h = -21 \rightarrow 31$
 $k = -7 \rightarrow 11$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.092$
 $S = 0.99$
4010 reflections
245 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0473P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.95 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.65 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

| | | | |
|-----------|-----------|--------|-----------|
| Au1–N1 | 2.025 (5) | Au1–P1 | 2.238 (2) |
| N1–Au1–P1 | 175.3 (2) | | |

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------|----------|-------------|-------------|---------------|
| O1–H1 \cdots N2 | 0.82 (8) | 2.09 (8) | 2.894 (8) | 168 (9) |

The phenyl rings of the triphenylphosphine ligand were refined as rigid hexagons ($C-C = 1.39 \text{ \AA}$). The H atoms were placed at calculated positions [aromatic $C-H = 0.93 \text{ \AA}$ and methyl $C-H = 0.96 \text{ \AA}$; $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$] and were included in the refinement in the riding-model approximation. The torsion angle of the methyl group was refined. The H atom belonging to the water O atom was located and refined freely.

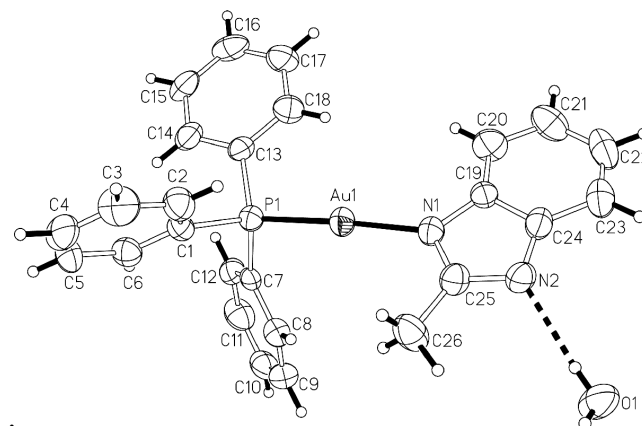


Figure 1

ORTEP II (Johnson, 1976) plot of the title compound (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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