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Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{N}-\text{C}) = 0.008 \text{ \AA}$
R factor = 0.040
wR factor = 0.108
Data-to-parameter ratio = 20.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Benzimidaxolyl(triphenylphosphine)gold(I)

The Au atom in the title compound, $[\text{Au}(\text{C}_7\text{H}_5\text{N}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$, displays linear coordination [$\text{Au}-\text{P} = 2.232(2) \text{ \AA}$, $\text{Au}-\text{N} = 2.022(5) \text{ \AA}$ and $\text{P}-\text{Au}-\text{N} = 179.6(1)^\circ$].

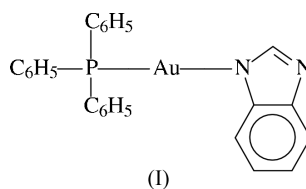
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Comment

This study extends our studies on electron-rich gold(I) complexes of triphenylphosphine (Chan *et al.*, 1994; Li *et al.*, 2002; Tzeng *et al.*, 1993). The title benzimidazolate complex, (I), (Fig. 1) exhibits photoluminescence (Wu, 2003), the origin of which probably cannot be explained from the crystal structure, as there are no significant intermolecular interactions. Similar compounds having a P/Au/N unit have been reported (Amagi *et al.*, 1989; Bonati *et al.*, 1985; Hao *et al.*, 2000; Nomiya *et al.*, 1998; Nomiya *et al.*, 2000; Nomiya, Noguchi, Ohsawa *et al.*, 2000). The bond dimensions involving the Au atom in the title complex compare well with those found in these other complexes [*e.g.* $\text{Au}-\text{P} = 2.232(2) \text{ \AA}$ and $\text{Au}-\text{N} = 2.024(7) \text{ \AA}$ in the pyrazolate, and $\text{Au}-\text{P} = 2.234(2) \text{ \AA}$ and $\text{Au}-\text{N} = 2.207(4) \text{ \AA}$ in the imidazolate].



Experimental

Triphenylphosphinechlorogold (0.99 g, 2.0 mmol) and benzimidazole (0.23 g, 2.0 mmol) were dissolved in acetone (20 ml). To this solution

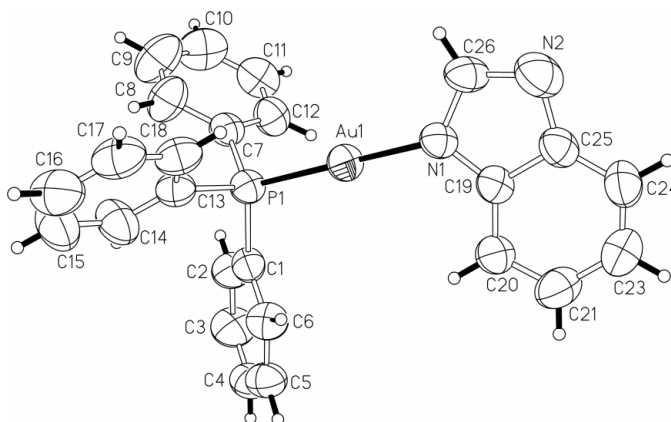


Figure 1

A view of (I), with displacement ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

was added 1 M sodium hydroxide (2 ml). Sodium chloride separated from the mixture when it was stirred for 2 h. The filtrate was evaporated to dryness and the crude product was dissolved in dichloromethane (10 ml). The compound was purified by recrystallization from dichloromethane/ether. Needle-shaped crystals were obtained in about 70% yield by the slow diffusion of ether into a dichloromethane solution of the compound. Analysis calculated for $C_{25}H_{20}AuN_2P$: C 52.09, H 3.50, N 4.86%; found: C 52.15, H 3.63, N 4.81%. IR (KBr, cm^{-1}): 3051 (w), 2924 (w), 1480 (w), 1465 (w), 1435 (s), 1295 (m), 1211 (m), 1161 (m), 1102 (s), 742 (s), 712 (m), 692 (s), 546 (s), 507 (m), 430 (w).

Crystal data

[Au(C₇H₅N₂)(C₁₈H₁₅P)]
 $M_r = 576.37$
 Triclinic, $P\bar{1}$
 $a = 6.5683$ (3) Å
 $b = 11.5851$ (4) Å
 $c = 15.1189$ (5) Å
 $\alpha = 103.011$ (1)°
 $\beta = 97.442$ (1)°
 $\gamma = 96.551$ (1)°
 $V = 1099.20$ (7) Å³
 $Z = 2$
 $D_x = 1.741$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 4902 reflections
 $\theta = 2.0$ – 26.4 °
 $\mu = 6.78$ mm⁻¹
 $T = 298$ (2) K
 Column, colorless
 $0.50 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 1999)
 $T_{min} = 0.122$, $T_{max} = 0.258$
 6827 measured reflections
 4433 independent reflections
 4022 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.038$
 $\theta_{max} = 26.4$ °
 $h = -8 \rightarrow 7$
 $k = -14 \rightarrow 14$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.108$
 $S = 1.03$
 4433 reflections
 214 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.3535P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 1.85$ e Å⁻³
 $\Delta\rho_{min} = -0.86$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Au1–N1	2.022 (5)	Au1–P1	2.232 (2)
N1–Au1–P1	179.6 (1)		

As the C–C distances of the phenyl rings deviated from the ideal value of 1.39 Å, these rings, as well as the benzene ring in the benzimidazolone group, were refined as rigid hexagons (C–C = 1.39 Å). H atoms were treated as riding [C–H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The final difference Fourier map had a large peak at about 1 Å from the Au atom.

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: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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