Acta Cryst. (1998). C**54**, 54–56

(2,3-Dioxoindolinyl-*N*)(triphenylphosphine-*P*)gold(I)

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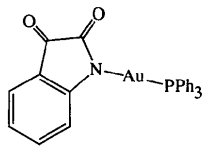
(*Received 29 April 1997; accepted 13 October 1997*)

Abstract

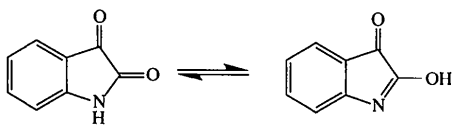
In the title compound, $[Au(C_8H_4NO_2)(C_{18}H_{15}P)]$, the $AuPPh_3$ group is located at the amino group. The Au—N and Au—P bond lengths are 2.047 (3) and 2.2461 (11) Å, respectively. In the crystal, indolinedione rings of two adjacent molecules related by an inversion centre have interplanar distances of 3.29 Å. Two short intermolecular Au···C distances (3.351 and 3.555 Å) are observed between the pairs of molecules.

Comment

The title compound, (1), represents the triphenylphosphinegold derivative of isatin, (2). Molecule (2) may exist in two tautomeric forms. Previously, X-ray diffraction studies have shown that molecule (2) exists only in the amino tautomeric form in the crystal (Goldschmidt & Llewellyn, 1950; Palmer, Blake & Gould, 1987; Frolova *et al.*, 1988; Palenik *et al.*, 1990). Molecule (1) is also potentially tautomeric. We were interested in the reason for the change in colour from yellow to red on transformation from isatin to its gold derivative.



(1)



(2)

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Molecule (1) exists in the amino tautomeric form. The Au—N bond distance of 2.047 (3) Å corresponds closely to those in other $AuPPh_3$ derivatives of arylamines, 2.038 (5) (Kuz'mina *et al.*, 1989), 2.050 (6) (Perevalova *et al.*, 1988) and 2.046 (9) Å (Kuz'mina *et al.*, 1990). The Au—P bond length of 2.2461 (11) Å is typical of Au^I compounds with a P—Au—N linear fragment (Kuz'mina, 1992). In the five-membered heterocyclic ring, bond distances reveal small but, we believe, significant differences from those found for (2) in the most precise investigation (Palenik *et al.*, 1990) and for *N*-methylisatin (3) (Miehe *et al.*, 1991). Both the N—C bonds and the C—C bond between the carbonyl groups [1.369 (5), 1.418 (5) and 1.577 (6) Å] are longer than the corresponding values in (2) [1.352 (3), 1.402 (3) and 1.555 (3) Å] and in (3) [1.353 (7), 1.407 (7) and 1.545 (7) Å]. The endocyclic C—N—C bond angle is 108.7 (3)° in (1), 110.4° in (3), and 111.8° in (2). The increase in the latter values correlates with the decrease in the positive inductive effect across the series $AuPPh_3 > CH_3 > H$. The positive inductive effect of the $AuPPh_3$ substituent at N, which causes some redistribution of electron density in the heterocycle of (1), may be responsible for the batochromism observed upon the replacement of H by $AuPPh_3$.

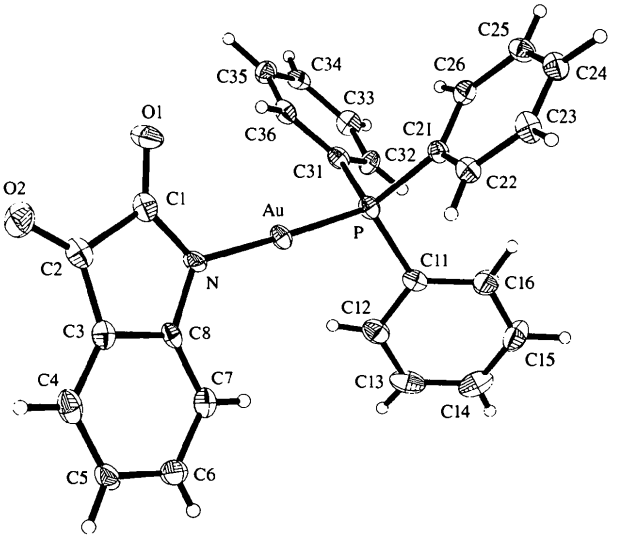

Fig. 1. The molecular structure of (1) showing 50% probability displacement ellipsoids.

Both C—O bonds [1.219 (5) and 1.224 (5) Å] lie within the ranges 1.206–1.220 and 1.196–1.211 Å characteristic of (2) and (3). The C1—C2 bond in (1) [1.577 (6) Å] is longer than in (2) and (3) [1.488–1.562 Å] and the C2—C3 bond in (1) [1.444 (6) Å] is shorter than in (2) and (3) [1.454–1.472 Å]. This bond-length analysis shows a rather significant bond-length redistribution in (1), caused by the $AuPPh_3$ substituent.

The molecules form pairwise stacks in the crystal (Fig. 2) and within each stack they are related by inversion. The mean interplanar distance is 3.29 Å; the shortest symmetrically independent intermolecular distances are: Au···C4^{i} 3.352 (4), Au···C5^{i} 3.555 (4), Cl···C7^{i} 3.329 (6), Cl···C6^{i} 3.407 (6) and C8···C8^{i} 3.319 (8) Å [symmetry code: (i) $-x$, $1-y$, $-z$]. These rather short distances allow us to suppose that the deep colour of (1) could also result from an intermolecular charge transfer within the stacks. Weak interactions between the Au atom and the multiple C—C bonds of an aromatic system have not been observed previously. Such interactions are known to be responsible for interesting photochemical and photophysical properties of Au^{I} compounds (Assefa, Staples & Fackler, 1994).

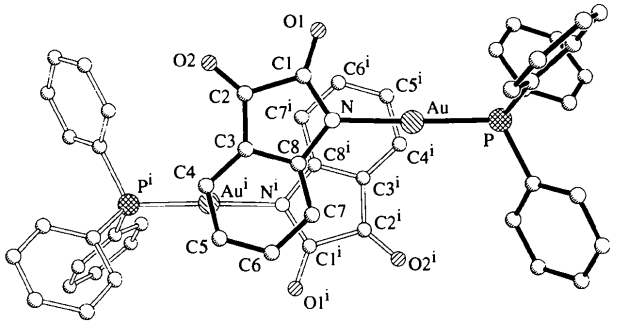

Fig. 2. View of the mode of overlap in the crystal. The reference molecule (solid bonds) is related to a second molecule (hollow bonds) by inversion through $(0, \frac{1}{2}, 0)$. [Symmetry code: (i) $-x$, $1-y$, $-z$.]

Experimental

The title compound was synthesized by reacting $[O(AuPPh_3)]BF_4$ (0.2 g, 0.14 mmol) with isatin (0.06 g, 0.41 mmol) in THF (15 ml) in the presence of aqueous potassium carbonate (0.1 g, 0.72 mmol) in H_2O (1 ml). In 5 min, the solution changed colour from yellow to bright red. Dark-red crystals were grown from THF.

Crystal data

$[Au(C_8H_4NO_2)(C_{18}H_{15}P)]$
M_r = 605.36
Monoclinic
$P2_1/c$
a = 9.2736 (2) Å
b = 11.4181 (2) Å
c = 20.5184 (3) Å
β = 93.696 (1)°
V = 2168.11 (7) Å^3
Z = 4
D_x = 1.855 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 15 515 reflections
θ = 1.99–27.48°
μ = 6.883 mm^{-1}
T = 153 (2) K
Plate
0.19 × 0.17 × 0.04 mm
Dark red

Data collection

Siemens SMART diffractometer
ω scans
Absorption correction: multi-scan (*SHELXTL*; Sheldrick, 1994)
T_{min} = 0.542, T_{max} = 0.746
15 515 measured reflections
4949 independent reflections
3866 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.48°
h = −12 → 11
k = −14 → 11
l = −26 → 26

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.070
S = 1.019
4749 reflections
357 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = −0.001
$\Delta\rho_{max}$ = 1.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.00078 (9)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Au—N	2.047 (3)	C2—C3	1.444 (6)
Au—P	2.2461 (11)	C3—C4	1.392 (6)
N—C1	1.369 (5)	C3—C8	1.409 (6)
N—C8	1.418 (5)	C4—C5	1.388 (7)
O1—C1	1.219 (5)	C5—C6	1.391 (7)
O2—C2	1.224 (5)	C6—C7	1.401 (6)
C1—C2	1.577 (6)	C7—C8	1.375 (6)
N—Au—P	177.08 (10)	C4—C3—C8	121.0 (4)
C1—N—C8	108.7 (3)	C4—C3—C2	132.1 (4)
C1—N—Au	124.4 (3)	C8—C3—C2	106.9 (4)
C8—N—Au	126.9 (3)	C5—C4—C3	118.4 (4)
O1—C1—N	128.3 (4)	C4—C5—C6	120.2 (4)
O1—C1—C2	124.6 (4)	C5—C6—C7	121.7 (5)
N—C1—C2	107.1 (4)	C8—C7—C6	118.0 (4)
O2—C2—C3	131.7 (4)	C7—C8—C3	120.6 (4)
O2—C2—C1	123.6 (4)	C7—C8—N	126.9 (4)
C3—C2—C1	104.8 (4)	C3—C8—N	112.5 (4)

All H atoms were found from difference Fourier synthesis and included in the least-squares refinement with individual isotropic displacement parameters. The largest peak in the difference electron-density map occurred 1.09 Å from Au.

Data collection: *SMART* (Siemens, 1995*a*). Cell refinement: *SAINT* (Siemens, 1995*b*). Data reduction: *SAINT*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL* (Sheldrick, 1994). Software used to prepare material for publication: *SHELXTL*.

This work was supported by Russian Foundation for Basic Research (project 95-03-08616a) and The Royal Society.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM1167). Services for accessing these data are described at the back of the journal.

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