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Trichlorido(2-phenylpyridine-κN)-gold(III)

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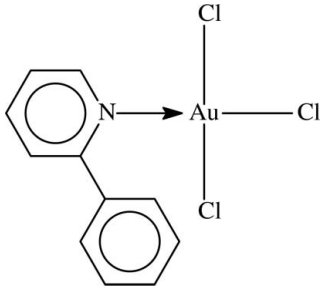
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.022; wR factor = 0.079; data-to-parameter ratio = 20.4.

The Au^{III} atom in the title compound, $[AuCl_3(C_{11}H_9N)]$, exists in a square planar $AuCl_3N$ geometry. The phenyl ring of the ligand is twisted by 51.6 (3)° with respect to the pyridyl ring.

Related literature

For the synthesis of the compound, see: Constable & Leese (1989). The compound is a precursor to (2-phenylpyridyl-κN,κC)gold(III) dichloride (Fan *et al.*, 2003).

For related literature, see: Zhang *et al.* (2006).



Experimental

Crystal data

$[AuCl_3(C_{11}H_9N)]$
M_r = 458.51
Triclinic, $P\overline{1}$
a = 8.192 (2) Å
b = 9.078 (2) Å
c = 10.296 (2) Å
α = 66.28 (3)°
β = 83.74 (3)°
γ = 68.02 (2)°
V = 649.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 11.92 mm^{-1}
T = 298 (2) K
0.29 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1995)
T_{min} = 0.090, T_{max} = 0.223
6439 measured reflections
2952 independent reflections
2823 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.079
S = 1.30
2952 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected bond lengths (Å).

Au1—N1	2.035 (5)	Au1—Cl2	2.258 (2)
Au1—Cl1	2.268 (2)	Au1—Cl3	2.280 (2)

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2395).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Constable, E. C. & Leese, T. A. (1989). *J. Organomet. Chem.* **363**, 419–424.
Fan, D., Yang, C.-T., Ranford, J. D., Lee, P. F. & Vittal, J. J. (2003). *J. Chem. Soc. Dalton Trans.* pp. 2680–2685.
Higashi, T. (1995). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Rigaku Corporation (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Westrip, S. P. (2007). *publCIF*. In preparation.
Zhang, X.-P., Yang, G. & Ng, S. W. (2006). *Acta Cryst.* E**62**, m2018–m2020.

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supplementary materials

Acta Cryst. (2007). E**63**, m1582 [**doi:10.1107/S1600536807021307**]

Trichlorido(2-phenylpyridine-*κN*)gold(III)

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Comment

A previous study reported the crystal structure of 4,4'-bipyridinium tetrachloroaurate(III) chloride, which was obtained unexpectedly from the reaction of 4,4'-bipyridine and potassium tetrachloraurate (Zhang *et al.*, 2006). The direct reaction of 2-phenylpyridine with gold chloride yielded the expected title compound (I), which has the metal center in a square plane that is composed of the donor nitrogen site along with three chlorine atoms (Table 1, Fig. 1).

Experimental

This compound was prepared as described in the literature (Constable & Leese, 1989). Bright-yellow crystals of (I) were obtained by its recrystalization from aqueous acetonitrile (xx:xx *v*/*v*).

Refinement

The H atoms were placed in calculated positions [C—H 0.93 Å; U(H) = 1.2U_{eq}(C)]. The highest peak in the final difference map is 0.9 Å from Au1 and the deepest hole is 0.7 Å from Au1.

Figures

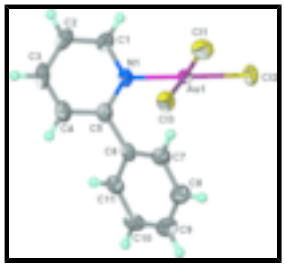

Fig. 1. **Figure 1**. View of the molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (arbitary spheres for the H atoms).

Trichlorido(2-phenylpyridine-κ*N*)gold(III)

Crystal data

$[AuCl_3(C_{11}H_9N)]$	$Z = 2$
$M_r = 458.51$	$F_{000} = 424$
Triclinic, $P\overline{1}$	$D_x = 2.346$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.192$ (2) Å	Cell parameters from 6137 reflections
$b = 9.078$ (2) Å	$\theta = 3.0$–$27.5°$
$c = 10.296$ (2) Å	$\mu = 11.92$ mm^{-1}

α = 66.28 (3)º	T = 298 (2) K
β = 83.74 (3)º	Block, yellow
γ = 68.02 (2)º	0.29 × 0.24 × 0.18 mm
V = 649.2 (2) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2952 independent reflections
Radiation source: fine-focus sealed tube	2823 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 298(2) K	θ_{max} = 27.5º
ω scan	θ_{min} = 3.0º
Absorption correction: mumerical (NUMABS; Higashi, 1995)	h = −10→10
T_{min} = 0.090, T_{max} = 0.223	k = −11→11
6439 measured reflections	l = −13→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.022	H-atom parameters constrained
$wR(F^2)$ = 0.079	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.2981P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.30	$(\Delta/\sigma)_{max}$ = 0.001
2952 reflections	$\Delta\rho_{max}$ = 1.06 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −0.92 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Au1	0.60793 (2)	0.81841 (2)	0.703793 (18)	0.03193 (9)
Cl1	0.4693 (2)	0.8672 (3)	0.8937 (2)	0.0564 (4)
Cl2	0.7651 (2)	0.9810 (2)	0.6926 (2)	0.0524 (4)
Cl3	0.7367 (2)	0.7757 (2)	0.50767 (17)	0.0468 (3)
N1	0.4665 (6)	0.6723 (6)	0.7124 (5)	0.0387 (10)
C1	0.2963 (7)	0.7577 (8)	0.6642 (7)	0.0450 (12)
H1	0.2464	0.8759	0.6421	0.054*
C2	0.1949 (8)	0.6762 (10)	0.6468 (7)	0.0528 (15)
H2	0.0772	0.7368	0.6151	0.063*
C3	0.2731 (10)	0.4994 (11)	0.6779 (8)	0.0597 (18)
H3	0.2095	0.4404	0.6642	0.072*
C4	0.4429 (9)	0.4153 (9)	0.7283 (7)	0.0519 (14)
H4	0.4949	0.2971	0.7512	0.062*

C5	0.5401 (8)	0.5015 (7)	0.7465 (6)	0.0406 (11)
C6	0.7262 (7)	0.4083 (7)	0.8082 (6)	0.0384 (11)
C7	0.7772 (8)	0.4233 (7)	0.9251 (6)	0.0435 (12)
H7	0.6982	0.4997	0.9619	0.052*
C8	0.9457 (9)	0.3244 (9)	0.9872 (8)	0.0527 (14)
H8	0.9791	0.3332	1.0664	0.063*
C9	1.0635 (9)	0.2131 (9)	0.9316 (8)	0.0563 (16)
H9	1.1768	0.1469	0.9728	0.068*
C10	1.0126 (9)	0.2001 (8)	0.8141 (8)	0.0532 (15)
H10	1.0924	0.1251	0.7765	0.064*
C11	0.8458 (8)	0.2966 (7)	0.7525 (7)	0.0470 (13)
H11	0.8131	0.2870	0.6734	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.03303 (12)	0.02905 (12)	0.03363 (13)	−0.00925 (8)	−0.00320 (8)	−0.01286 (8)
Cl1	0.0579 (9)	0.0643 (10)	0.0499 (9)	−0.0134 (8)	0.0078 (7)	−0.0345 (8)
Cl2	0.0608 (9)	0.0451 (7)	0.0611 (10)	−0.0273 (7)	−0.0070 (7)	−0.0205 (7)
Cl3	0.0538 (8)	0.0525 (8)	0.0415 (8)	−0.0237 (7)	0.0098 (6)	−0.0235 (6)
N1	0.042 (2)	0.045 (2)	0.037 (2)	−0.023 (2)	0.0048 (19)	−0.018 (2)
C1	0.040 (3)	0.054 (3)	0.043 (3)	−0.018 (3)	0.000 (2)	−0.020 (3)
C2	0.040 (3)	0.076 (4)	0.049 (4)	−0.029 (3)	0.000 (3)	−0.024 (3)
C3	0.072 (4)	0.077 (5)	0.060 (4)	−0.053 (4)	0.010 (3)	−0.034 (4)
C4	0.063 (4)	0.047 (3)	0.054 (4)	−0.030 (3)	−0.002 (3)	−0.018 (3)
C5	0.051 (3)	0.044 (3)	0.032 (3)	−0.023 (2)	0.001 (2)	−0.014 (2)
C6	0.048 (3)	0.034 (2)	0.040 (3)	−0.023 (2)	0.004 (2)	−0.014 (2)
C7	0.050 (3)	0.042 (3)	0.033 (3)	−0.012 (2)	−0.002 (2)	−0.013 (2)
C8	0.051 (3)	0.056 (4)	0.049 (4)	−0.015 (3)	−0.005 (3)	−0.020 (3)
C9	0.050 (3)	0.053 (4)	0.056 (4)	−0.014 (3)	−0.001 (3)	−0.015 (3)
C10	0.056 (3)	0.040 (3)	0.055 (4)	−0.008 (3)	0.003 (3)	−0.019 (3)
C11	0.055 (3)	0.041 (3)	0.050 (3)	−0.015 (3)	0.002 (3)	−0.024 (3)

Geometric parameters (Å, °)

Au1—N1	2.035 (5)	C4—H4	0.9300
Au1—Cl1	2.268 (2)	C5—C6	1.503 (8)
Au1—Cl2	2.258 (2)	C6—C7	1.388 (8)
Au1—Cl3	2.280 (2)	C6—C11	1.385 (8)
N1—C1	1.351 (8)	C7—C8	1.387 (9)
N1—C5	1.341 (7)	C7—H7	0.9300
C1—C2	1.367 (8)	C8—C9	1.377 (10)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.397 (11)	C9—C10	1.382 (10)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.353 (10)	C10—C11	1.372 (9)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.378 (8)	C11—H11	0.9300

N1—Au1—Cl1	90.2 (1)	N1—C5—C4	119.8 (6)
N1—Au1—Cl2	179.6 (1)	N1—C5—C6	118.5 (5)
N1—Au1—Cl3	88.9 (1)	C4—C5—C6	121.7 (5)
Cl1—Au1—Cl2	90.21 (7)	C7—C6—C11	119.5 (6)
Cl1—Au1—Cl3	177.68 (5)	C7—C6—C5	121.4 (5)
Cl2—Au1—Cl3	90.70 (6)	C11—C6—C5	118.9 (5)
C1—N1—C5	119.8 (5)	C6—C7—C8	120.1 (6)
C1—N1—Au1	116.8 (4)	C6—C7—H7	120.0
C5—N1—Au1	122.9 (4)	C8—C7—H7	120.0
N1—C1—C2	122.2 (6)	C9—C8—C7	120.0 (7)
N1—C1—H1	118.9	C9—C8—H8	120.0
C2—C1—H1	118.9	C7—C8—H8	120.0
C1—C2—C3	118.1 (6)	C10—C9—C8	119.7 (6)
C1—C2—H2	121.0	C10—C9—H9	120.2
C3—C2—H2	121.0	C8—C9—H9	120.2
C4—C3—C2	119.0 (6)	C9—C10—C11	120.8 (6)
C4—C3—H3	120.5	C9—C10—H10	119.6
C2—C3—H3	120.5	C11—C10—H10	119.6
C3—C4—C5	121.2 (6)	C10—C11—C6	119.9 (6)
C3—C4—H4	119.4	C10—C11—H11	120.0
C5—C4—H4	119.4	C6—C11—H11	120.0
Cl1—Au1—N1—C1	75.5 (4)	C3—C4—C5—C6	177.4 (6)
Cl3—Au1—N1—C1	−102.4 (4)	N1—C5—C6—C7	52.6 (7)
Cl1—Au1—N1—C5	−112.9 (4)	C4—C5—C6—C7	−125.4 (6)
Cl3—Au1—N1—C5	69.3 (4)	N1—C5—C6—C11	−131.6 (6)
C5—N1—C1—C2	−0.9 (9)	C4—C5—C6—C11	50.3 (8)
Au1—N1—C1—C2	171.1 (5)	C11—C6—C7—C8	−1.2 (8)
N1—C1—C2—C3	−1.2 (10)	C5—C6—C7—C8	174.5 (5)
C1—C2—C3—C4	2.3 (10)	C6—C7—C8—C9	1.0 (10)
C2—C3—C4—C5	−1.4 (11)	C7—C8—C9—C10	−0.2 (10)
C1—N1—C5—C4	1.8 (8)	C8—C9—C10—C11	−0.2 (10)
Au1—N1—C5—C4	−169.6 (5)	C9—C10—C11—C6	−0.1 (10)
C1—N1—C5—C6	−176.3 (5)	C7—C6—C11—C10	0.8 (9)
Au1—N1—C5—C6	12.3 (7)	C5—C6—C11—C10	−175.0 (5)
C3—C4—C5—N1	−0.7 (10)		

Fig. 1