3-Phenylpyridinium tetrachlorido-aurate(III)

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In the title molecular salt, $(C_{11}H_{10}N)[AuCl_4]$, the Au^{III} atom adopts an almost regular square-planar coordination geometry and the dihedral angle between the aromatic rings of the 3-phenylpyridinium cation is 23.1 (3)°. In the crystal, the ions interact by way of N—H⋯Cl and C—H⋯Cl hydrogen bonds.

Related literature

For related structures, see: Calleja *et al.* (2001); Fazaeli *et al.* (2010); Hasan *et al.* (1999); Hojjat Kashani *et al.* (2008); Johnson & Steed (1998); Safari *et al.* (2009); Yap *et al.* (1995); Yıldırım, Akkurt, Safari, Abedi *et al.* (2009); Yıldırım, Akkurt, Safari, Amani & McKee (2009); Zhang *et al.* (2006).

Experimental

Crystal data

$(C_{11}H_{10}N)[AuCl_4]$	$\gamma = 97.216\,(10)°$
$M_r = 494.97$	$V = 694.20\,(15)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 7.7629\,(9)$ Å	Mo $K\alpha$ radiation
$b = 8.5901\,(11)$ Å	$\mu = 11.34$ mm^{-1}
$c = 11.0530\,(15)$ Å	$T = 298$ K
$\alpha = 94.106\,(11)°$	$0.40 \times 0.35 \times 0.28$ mm
$\beta = 107.125\,(10)°$	

Data collection

Stoe IPDSII diffractometer	7980 measured reflections
Absorption correction: numerical	3688 independent reflections
(X-RED; Stoe & Cie, 2005)	3513 reflections with $I > 2\sigma(I)$
$T_{min} = 0.067$, $T_{max} = 0.180$	$R_{int} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	154 parameters
$wR(F^2) = 0.083$	H-atom parameters constrained
$S = 1.15$	$\Delta\rho_{max} = 1.19$ e Å^{-3}
3688 reflections	$\Delta\rho_{min} = -1.85$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Au1—Cl2	2.2740 (13)	Au1—Cl1	2.2762 (12)
Au1—Cl3	2.2754 (12)	Au1—Cl4	2.2766 (13)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯Cl3^i	0.86	2.63	3.359 (7)	143
C1—H1⋯Cl4^i	0.93	2.83	3.755 (7)	175

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

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S1. Comment

There are several proton transfer systems using $HAuCl_4$ with proton acceptor molecules, such as $[EMI][AuCl_4]$, (II) and $[BMI]_2[AuCl_4].2H_2O$, (III), (Hasan *et al.*, 1999), $[H_2bipy][AuCl_4][Cl]$, (IV), (Zhang *et al.*, 2006), $[H_7O_3][15\text{-crown-}5]$ $[AuCl_4]$, (V) and $[H_5O_2][benzo\text{-}15\text{-crown-}5]_2[AuCl_4]$, (VI), (Johnson & Steed, 1998), $[H_5O_2]_2[12\text{-crown-}4]_2[AuCl_4]_2$, (VII), $[H_3O][18\text{-crown-}6][AuCl_4]$, (VIII) and $[H_3O][4\text{-nitrobenzo-}18\text{-crown-}6][AuCl_4]$, (IX), (Calleja *et al.*, 2001), $[DPpy.H][AuCl_4]$, (X), (Yap *et al.*, 1995),$[H_2DA18C6][AuCl_4].2H2O$, (XI), (Hojjat Kashani *et al.*, 2008), $[dafonium]$ $[dafone][AuCl_4]$, (XII), (Safari *et al.*, 2009), $[pz(py)_2.H][AuCl_4]$, (XIII), (Yıldırım, Akkurt, Safari, Amani & McKee 2009), $[Ph_2Phen.H][AuCl_4]$, (XIV), (Yıldırım, Akkurt, Safari, Abedi *et al.*, 2009) and $[TBA]_2[AuCl_4][Cl]$, (XV), (Fazaeli *et al.*, 2010) [Where EMI is 1-ethyl-3-methylimidazolium, BMI is 1-butyl-3-methylimidazolium, H_2bipy is 2,2′-bipyridinium, DPpy.H is 2,6-diphenylpyridinium, H_2DA18C6 is 1,10-diazonia-18-crown-6, dafonium is 9-oxo-4,5-diaza-fluoren-4-ium, dafone is 4,5-diazafluoren-9-one, $pz(py)_2$.H is 2-(3-pyridin-2-ylpyrazin-2-yl)pyridinium, Ph_2Phen.H is 2,9-dimethyl-4,7-diphenyl-1,10-phenanthrolin-1-ium and TBA is tribenzylammonium] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

The molecule of the title compound, (I), (Fig. 1), contains one independent protonated 3-phenylpyridinium cation and one $[AuCl_4]^-$ anion. The Au^{III} atom has a squareplanar environment defined by four Cl atoms. In $[AuCl_4]^-$ anion, the Au—Cl bond lengths and angles (Table 1) are within normal range (II, III, VII, VIII and IX).

In the crystal structure, intermolecular N—H···Cl and C—H···Cl hydrogen bonds (Table 2) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure.

S2. Experimental

A solution of 3-phenylpyridine (0.11 g, 0.09 ml, 0.74 mmol) in methanol (5 ml) was added to a solution of $HAuCl_4.3H_2O$, (0.29 g, 0.74 mmol) in acetonitrile (15 ml) and the resulting yellow solution was stirred for 30 min at 313 K. Then, it was left to evaporate slowly at room temperature. After five days, yellow blocks of (I) were isolated (yield 0.26 g; 71.0%).

S3. Refinement

All H atoms were positioned geometrically, with C—H=0.93Å for aromatics H and constrained to ride on their parent atoms, with $U_{iso}(H)=1.2U_{eq}$.
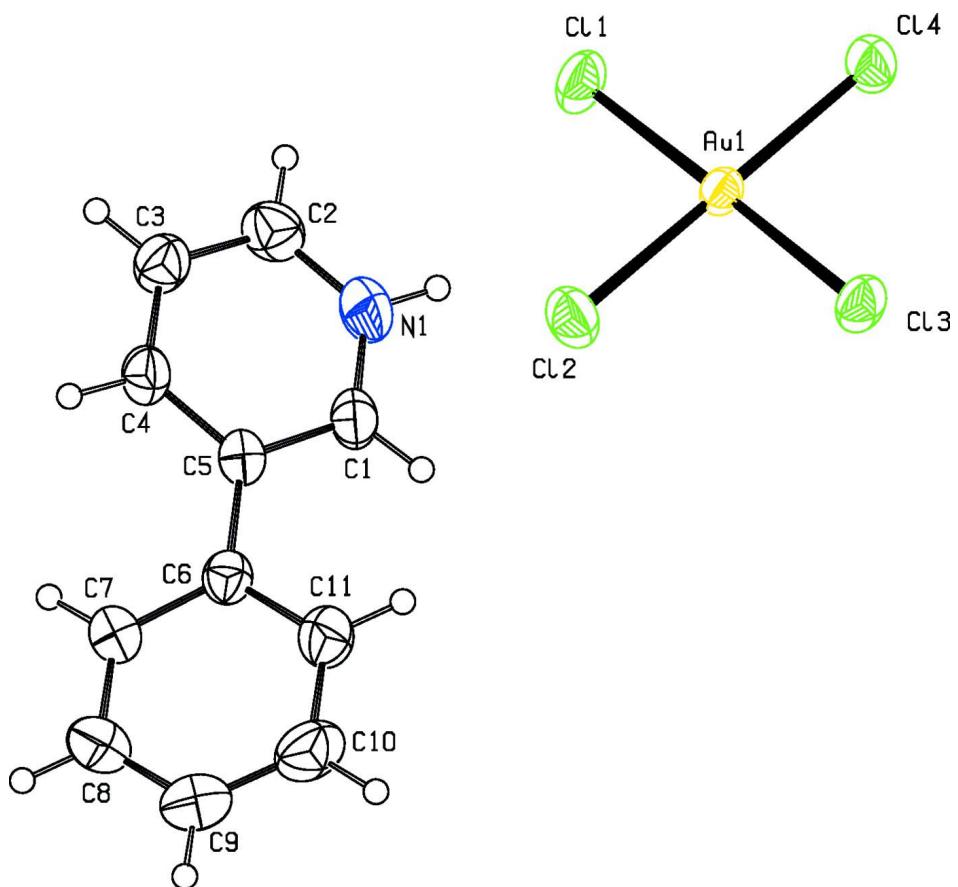
Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 40% probability level.
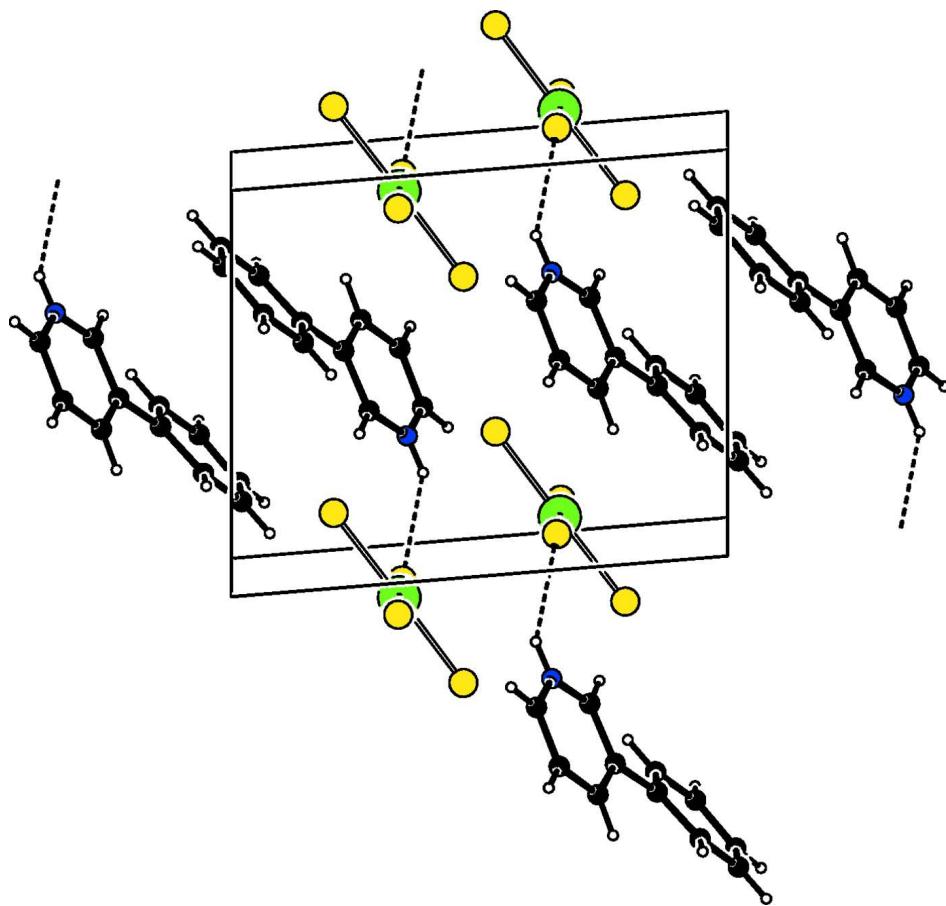
Figure 2

Unit-cell packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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Crystal data
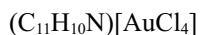
$(C_{11}H_{10}N)[AuCl_4]$	$Z = 2$
$M_r = 494.97$	$F(000) = 460$
Triclinic, $P\bar{1}$	$D_x = 2.368$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.7629$ (9) Å	Cell parameters from 984 reflections
$b = 8.5901$ (11) Å	$\theta = 1.9$–$29.2°$
$c = 11.0530$ (15) Å	$\mu = 11.34$ mm^{-1}
$\alpha = 94.106$ (11)°	$T = 298$ K
$\beta = 107.125$ (10)°	Block, yellow
$\gamma = 97.216$ (10)°	$0.40 \times 0.35 \times 0.28$ mm
$V = 694.20$ (15) Å^3	

Data collection

Stoe IPDS II diffractometer	Absorption correction: numerical (*X-RED*; Stoe & Cie, 2005)
Radiation source: fine-focus sealed tube	$T_{min} = 0.067$, $T_{max} = 0.180$
Graphite monochromator	7980 measured reflections
Detector resolution: 0.15 mm pixels mm^{-1}	3688 independent reflections
rotation method scans	3513 reflections with $I > 2\sigma(I)$

$R_{int} = 0.051$

$\theta_{max} = 29.2°$, $\theta_{min} = 1.9°$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.083$	
$S = 1.15$	H-atom parameters constrained
3688 reflections	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.4225P]$
154 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 1.19$ e Å^{-3}
	$\Delta\rho_{min} = -1.85$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
C1	0.3073 (8)	0.3645 (7)	0.7222 (6)	0.0534 (13)
H1	0.4141	0.3203	0.7415	0.064*
C2	−0.0102 (9)	0.3328 (8)	0.6148 (7)	0.0593 (14)
H2	−0.1157	0.2683	0.5638	0.071*
C3	−0.0149 (8)	0.4824 (7)	0.6606 (6)	0.0556 (13)
H3	−0.1242	0.5229	0.6395	0.067*
C4	0.1433 (8)	0.5748 (6)	0.7388 (6)	0.0487 (11)
H4	0.1386	0.6775	0.7691	0.058*
C5	0.3102 (7)	0.5176 (6)	0.7733 (5)	0.0412 (9)
C6	0.4797 (7)	0.6118 (6)	0.8579 (5)	0.0429 (9)
C7	0.4751 (9)	0.7355 (7)	0.9442 (6)	0.0556 (13)
H7	0.3628	0.7566	0.9497	0.067*
C8	0.6310 (11)	0.8273 (9)	1.0215 (7)	0.0693 (18)
H8	0.6239	0.9105	1.0776	0.083*
C9	0.7981 (10)	0.7962 (10)	1.0160 (7)	0.0676 (17)
H9	0.9042	0.8600	1.0669	0.081*
C10	0.8084 (9)	0.6706 (10)	0.9353 (8)	0.0721 (19)
H10	0.9217	0.6470	0.9342	0.087*
C11	0.6485 (8)	0.5781 (8)	0.8545 (6)	0.0591 (14)
H11	0.6556	0.4944	0.7989	0.071*
N1	0.1525 (9)	0.2805 (7)	0.6455 (6)	0.0651 (14)
H1A	0.1565	0.1871	0.6136	0.078*

Au1	0.377224 (19)	0.071414 (17)	0.338315 (15)	0.03590 (7)
Cl1	0.08562 (18)	0.08586 (18)	0.33626 (17)	0.0559 (3)
Cl2	0.4746 (2)	0.30376 (17)	0.46750 (16)	0.0571 (3)
Cl3	0.67028 (17)	0.05728 (17)	0.34422 (16)	0.0509 (3)
Cl4	0.28061 (19)	−0.15918 (17)	0.20634 (17)	0.0581 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.051 (3)	0.046 (3)	0.063 (3)	0.013 (2)	0.019 (2)	−0.006 (2)
C2	0.056 (3)	0.052 (3)	0.064 (3)	−0.004 (2)	0.016 (3)	−0.002 (3)
C3	0.046 (3)	0.052 (3)	0.067 (3)	0.008 (2)	0.016 (2)	0.004 (3)
C4	0.053 (3)	0.039 (2)	0.057 (3)	0.012 (2)	0.019 (2)	0.003 (2)
C5	0.047 (2)	0.037 (2)	0.045 (2)	0.0093 (18)	0.0195 (19)	0.0048 (17)
C6	0.046 (2)	0.042 (2)	0.044 (2)	0.0103 (18)	0.0162 (19)	0.0077 (18)
C7	0.057 (3)	0.054 (3)	0.053 (3)	0.013 (2)	0.014 (2)	−0.005 (2)
C8	0.072 (4)	0.066 (4)	0.057 (3)	0.009 (3)	0.004 (3)	−0.010 (3)
C9	0.053 (3)	0.078 (4)	0.064 (4)	0.005 (3)	0.007 (3)	0.011 (3)
C10	0.042 (3)	0.098 (5)	0.075 (4)	0.012 (3)	0.016 (3)	0.011 (4)
C11	0.050 (3)	0.066 (3)	0.064 (3)	0.012 (3)	0.023 (3)	−0.001 (3)
N1	0.071 (3)	0.045 (2)	0.074 (3)	0.011 (2)	0.018 (3)	−0.011 (2)
Au1	0.02898 (10)	0.03416 (10)	0.04446 (11)	0.00715 (6)	0.01061 (7)	0.00261 (7)
Cl1	0.0343 (5)	0.0527 (6)	0.0830 (9)	0.0122 (5)	0.0208 (6)	0.0012 (6)
Cl2	0.0560 (7)	0.0460 (6)	0.0653 (8)	0.0017 (5)	0.0195 (6)	−0.0122 (6)
Cl3	0.0307 (5)	0.0498 (6)	0.0711 (8)	0.0074 (4)	0.0153 (5)	−0.0007 (6)
Cl4	0.0428 (6)	0.0492 (6)	0.0737 (9)	0.0055 (5)	0.0108 (6)	−0.0164 (6)

Geometric parameters (Å, º)

C1—N1	1.333 (8)	C7—H7	0.9300
C1—C5	1.389 (7)	C8—C9	1.375 (12)
C1—H1	0.9300	C8—H8	0.9300
C2—N1	1.351 (9)	C9—C10	1.376 (11)
C2—C3	1.356 (9)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.403 (9)
C3—C4	1.384 (8)	C10—H10	0.9300
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.400 (7)	N1—H1A	0.8600
C4—H4	0.9300	Au1—Cl2	2.2740 (13)
C5—C6	1.470 (8)	Au1—Cl3	2.2754 (12)
C6—C11	1.388 (8)	Au1—Cl1	2.2762 (12)
C6—C7	1.388 (7)	Au1—Cl4	2.2766 (13)
C7—C8	1.368 (9)		
N1—C1—C5	120.5 (5)	C7—C8—C9	119.8 (7)
N1—C1—H1	119.7	C7—C8—H8	120.1
C5—C1—H1	119.7	C9—C8—H8	120.1
N1—C2—C3	117.9 (6)	C8—C9—C10	120.0 (7)

N1—C2—H2	121.0	C8—C9—H9	120.0
C3—C2—H2	121.0	C10—C9—H9	120.0
C2—C3—C4	119.9 (6)	C9—C10—C11	120.2 (6)
C2—C3—H3	120.0	C9—C10—H10	119.9
C4—C3—H3	120.0	C11—C10—H10	119.9
C3—C4—C5	121.7 (5)	C6—C11—C10	119.8 (6)
C3—C4—H4	119.2	C6—C11—H11	120.1
C5—C4—H4	119.2	C10—C11—H11	120.1
C1—C5—C4	115.8 (5)	C1—N1—C2	124.0 (5)
C1—C5—C6	121.2 (5)	C1—N1—H1A	118.0
C4—C5—C6	123.0 (4)	C2—N1—H1A	118.0
C11—C6—C7	118.3 (5)	Cl2—Au1—Cl3	89.51 (5)
C11—C6—C5	120.8 (5)	Cl2—Au1—Cl1	89.92 (6)
C7—C6—C5	120.8 (5)	Cl3—Au1—Cl1	178.98 (5)
C8—C7—C6	121.8 (6)	Cl2—Au1—Cl4	179.07 (6)
C8—C7—H7	119.1	Cl3—Au1—Cl4	90.20 (5)
C6—C7—H7	119.1	Cl1—Au1—Cl4	90.38 (5)
N1—C2—C3—C4	−1.5 (10)	C11—C6—C7—C8	2.5 (10)
C2—C3—C4—C5	−0.5 (10)	C5—C6—C7—C8	−178.3 (6)
N1—C1—C5—C4	−0.2 (9)	C6—C7—C8—C9	−1.0 (12)
N1—C1—C5—C6	−180.0 (6)	C7—C8—C9—C10	−1.6 (13)
C3—C4—C5—C1	1.3 (9)	C8—C9—C10—C11	2.7 (12)
C3—C4—C5—C6	−178.9 (5)	C7—C6—C11—C10	−1.4 (10)
C1—C5—C6—C11	23.1 (8)	C5—C6—C11—C10	179.4 (6)
C4—C5—C6—C11	−156.7 (6)	C9—C10—C11—C6	−1.1 (12)
C1—C5—C6—C7	−156.1 (6)	C5—C1—N1—C2	−1.9 (11)
C4—C5—C6—C7	24.1 (8)	C3—C2—N1—C1	2.8 (11)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯Cl3[i]	0.86	2.63	3.359 (7)	143
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