

3-Phenylpyridinium tetrachloridoaurate(III)

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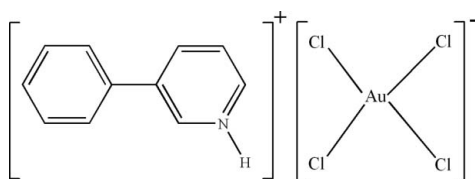
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å;
 R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 23.9.

In the title molecular salt, $(\text{C}_{11}\text{H}_{10}\text{N})[\text{AuCl}_4]$, 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 $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{Cl}$ 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

$(\text{C}_{11}\text{H}_{10}\text{N})[\text{AuCl}_4]$
 $M_r = 494.97$
Triclinic, $P\bar{1}$
 $a = 7.7629$ (9) Å
 $b = 8.5901$ (11) Å
 $c = 11.0530$ (15) Å
 $\alpha = 94.106$ (11)°
 $\beta = 107.125$ (10)°

$\gamma = 97.216$ (10)°
 $V = 694.20$ (15) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 11.34$ mm⁻¹
 $T = 298$ K
 $0.40 \times 0.35 \times 0.28$ mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical
(*X-RED*; Stoe & Cie, 2005)
 $T_{\min} = 0.067$, $T_{\max} = 0.180$

7980 measured reflections
3688 independent reflections
3513 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.083$
 $S = 1.15$
3688 reflections

154 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.19$ e Å⁻³
 $\Delta\rho_{\min} = -1.85$ 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, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{Cl3}^{\text{i}}$	0.86	2.63	3.359 (7)	143
$\text{C1}-\text{H1}\cdots\text{Cl4}^{\text{i}}$	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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5341).

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supplementary materials

Acta Cryst. (2010). E66, m345 [doi:10.1107/S1600536810006860]

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Comment

There are several proton transfer systems using HAuCl_4 with proton acceptor molecules, such as $[\text{EMI}][\text{AuCl}_4]$, (II) and $[\text{BMI}]_2[\text{AuCl}_4] \cdot 2\text{H}_2\text{O}$, (III), (Hasan *et al.*, 1999), $[\text{H}_2\text{bipy}][\text{AuCl}_4][\text{Cl}]$, (IV), (Zhang *et al.*, 2006), $[\text{H}_7\text{O}_3][15\text{-crown-5}][\text{AuCl}_4]$, (V) and $[\text{H}_5\text{O}_2][\text{benzo-15-crown-5}]_2[\text{AuCl}_4]$, (VI), (Johnson & Steed, 1998), $[\text{H}_5\text{O}_2]_2[12\text{-crown-4}]_2[\text{AuCl}_4]_2$, (VII), $[\text{H}_3\text{O}][18\text{-crown-6}][\text{AuCl}_4]$, (VIII) and $[\text{H}_3\text{O}][4\text{-nitrobenzo-18-crown-6}][\text{AuCl}_4]$, (IX), (Calleja *et al.*, 2001), $[\text{DPPy.H}][\text{AuCl}_4]$, (X), (Yap *et al.*, 1995), $[\text{H}_2\text{DA18C6}][\text{AuCl}_4] \cdot 2\text{H}_2\text{O}$, (XI), (Hojjat Kashani *et al.*, 2008), $[\text{dafonium}][\text{dafone}][\text{AuCl}_4]$, (XII), (Safari *et al.*, 2009), $[\text{pz}(\text{py})_2.\text{H}][\text{AuCl}_4]$, (XIII), (Yıldırım, Akkurt, Safari, Amani & McKee 2009), $[\text{Ph}_2\text{Phen.H}][\text{AuCl}_4]$, (XIV), (Yıldırım, Akkurt, Safari, Abedi *et al.*, 2009) and $[\text{TBA}]_2[\text{AuCl}_4][\text{Cl}]$, (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, $\text{H}_2\text{DA18C6}$ is 1,10-diazonia-18-crown-6, dafonium is 9-oxo-4,5-diazafluoren-4-ium, dafone is 4,5-diazafluoren-9-one, $\text{pz}(\text{py})_2.\text{H}$ is 2-(3-pyridin-2-ylpyrazin-2-yl)pyridinium, $\text{Ph}_2\text{Phen.H}$ is 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline-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 $[\text{AuCl}_4]^-$ anion. The Au^{III} atom has a squareplanar environment defined by four Cl atoms. In $[\text{AuCl}_4]^-$ 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 \cdots Cl and C—H \cdots Cl hydrogen bonds (Table 2) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure.

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 $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$, (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%).

Refinement

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

Figures

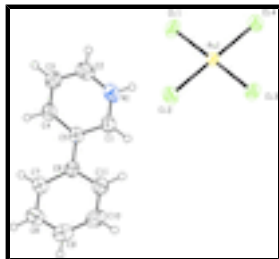


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 40% probability level.

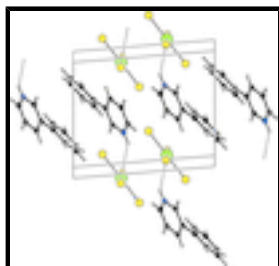


Fig. 2. Unit-cell packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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Crystal data

(C₁₁H₁₀N)[AuCl₄]

M_r = 494.97

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

a = 7.7629 (9) Å

b = 8.5901 (11) Å

c = 11.0530 (15) Å

α = 94.106 (11)°

β = 107.125 (10)°

γ = 97.216 (10)°

V = 694.20 (15) Å³

Z = 2

F(000) = 460

D_x = 2.368 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 984 reflections

θ = 1.9–29.2°

μ = 11.34 mm⁻¹

T = 298 K

Block, yellow

0.40 × 0.35 × 0.28 mm

Data collection

Stoe IPDS II
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 0.15 mm pixels mm⁻¹
rotation method scans

Absorption correction: numerical
(X-RED; Stoe & Cie, 2005)

T_{min} = 0.067, *T_{max}* = 0.180

7980 measured reflections

3688 independent reflections

3513 reflections with *I* > 2σ(*I*)

R_{int} = 0.051

θ_{\max} = 29.2°, θ_{\min} = 1.9°

h = -10→10

k = -11→11

l = -15→15

Refinement

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

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

supplementary materials

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 (\AA^2)

	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 (\AA , $^\circ$)

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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots Cl3 ⁱ	0.86	2.63	3.359 (7)	143
C1—H1 \cdots Cl4 ⁱ	0.93	2.83	3.755 (7)	175

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

Fig. 1

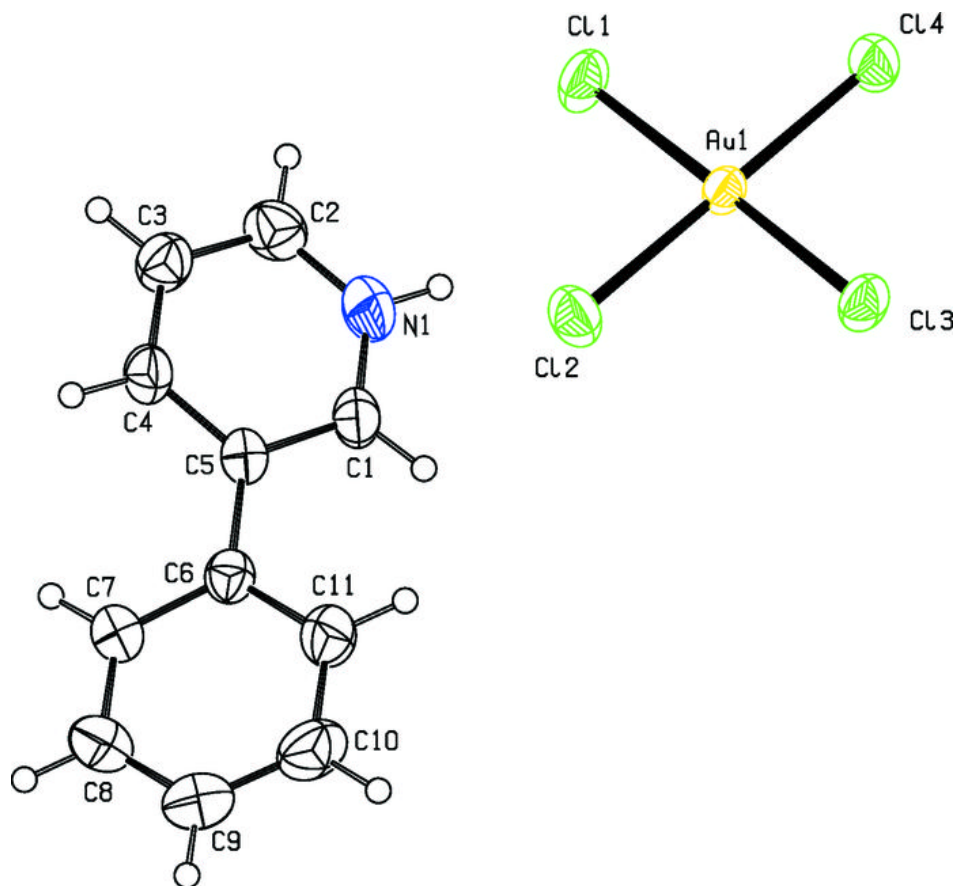


Fig. 2

