

Bis(2,6-dimethylpyridine- κ N)gold(I) tetrachloridoaurate(III)

Roya Ahmadi,^a Leila Dehghan,^a Vahid Amani^{a*} and Hamid Reza Khavasi^b

^aIslamic Azad University, Shahr-e-Rey Branch, Tehran, Iran, and ^bDepartment of Chemistry, Shahid Beheshti University, Tehran 1983963113, Iran

Correspondence e-mail: v_amani2002@yahoo.com

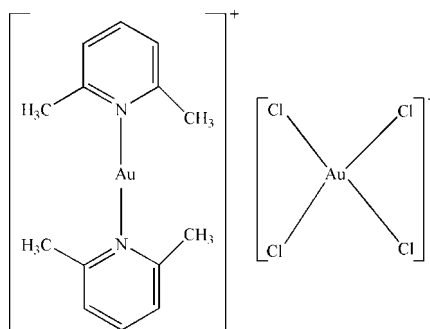
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.019$ Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 20.1.

In the cation of the title compound, $[\text{Au}(\text{C}_7\text{H}_9\text{N})_2][\text{AuCl}_4]$, the Au^{I} atom is two-coordinated in a linear arrangement by two N atoms from two 2,6-dimethylpyridine ligands. In the anion, the Au^{III} atom has a virtually square-planar coordination geometry. The Au atoms both are located on centers of inversion. The crystal structure involves intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Related literature

For related literature, see: Abbate *et al.* (2000); Adams & Strähle (1982); Ahmadi *et al.* (2008); Amani *et al.* (2008); Bjernemose *et al.* (2004); Hayoun *et al.* (2006); Hojjat Kashani *et al.* (2008); Hollis & Lippard (1983); McInnes *et al.* (1995); Yildirim *et al.* (2008).



Experimental

Crystal data

$[\text{Au}(\text{C}_7\text{H}_9\text{N})_2][\text{AuCl}_4]$
 $M_r = 750.04$

Monoclinic, $C2/m$
 $a = 17.773$ (3) Å
 $b = 6.8395$ (8) Å
 $c = 8.3728$ (14) Å
 $\beta = 110.929$ (12)°

$V = 950.6$ (3) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 15.97$ mm⁻¹
 $T = 298$ (2) K
 $0.20 \times 0.12 \times 0.08$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.112$, $T_{\text{max}} = 0.275$

5473 measured reflections
1384 independent reflections
1123 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.092$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.115$
 $S = 1.20$
1384 reflections

69 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.76$ e Å⁻³
 $\Delta\rho_{\text{min}} = -2.1$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Au1—N1	2.030 (8)	Au2—Cl2	2.286 (4)
Au2—Cl1	2.280 (3)		
Cl1 ⁱ —Au2—Cl2	90.05 (14)	Cl1—Au2—Cl2	89.95 (14)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots Cl1 ⁱⁱ	0.93	2.77	3.572 (14)	145

Symmetry code: (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + 2$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HY2150).

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supplementary materials

Acta Cryst. (2008). E64, m1237 [doi:10.1107/S1600536808027876]

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Comment

Recently, we reported the syntheses and crystal structures of [Au(dmphen)Cl₂][AuCl₄], (II), (Ahmadi *et al.*, 2008), [dmpyH][PtCl₆], (III), (Amani *et al.*, 2008) and [H₂DA18C6][AuCl₄].2H₂O, (IV), (Hojjat Kashani *et al.*, 2008) (dmphen = 4,7-diphenyl-1,10-phenanthroline; dmpyH = 2,6-dimethylpyridinium and H₂DA18C6 = 1,10-diazonia-18-crown-6). Several Au^{III} complexes with formula [AuCl₂L]₂X, such as [AuCl₂(bipy)](BF₄), (V), (McInnes *et al.*, 1995), [AuCl₂(bipy)](NO₃), (VI), (Bjernemose *et al.*, 2004), [AuCl₂(bipy)][AuBr₄], (VII), (Hayoun *et al.*, 2006), [AuCl₂(dtbpy)][AuCl₄].CH₃CN, (VIII), (Yildirim *et al.*, 2008) and [AuCl₂(phen)Cl].H₂O, (IX), (Abbate *et al.*, 2000) (bipy = 2,2'-bipyridine; dtbpy = 4,4'-ditertbutyl-2,2'-bipyridine; phen = 1,10-phenanthroline) have been synthesized and characterized by single-crystal X-ray diffraction methods. Two Au^{III} complexes with formula [AuCl₂L₂]₂X, [AuCl₂(py)₂][AuCl₄], (X), and [AuCl₂(py)₂Cl].H₂O, (XI), (Adams & Strahle, 1982) (py = pyridine) and only one mixed-valence Au^I-Au^{III} complex, [Au(terpy)Cl]₂[AuCl₂]₃[AuCl₄], (XII), (Hollis & Lippard, 1983) (terpy = 2,2',2''-terpyridine) 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).

In the cation of the title compound (Fig. 1), the Au^I atom is two-coordinated in a linear arrangement by two N atoms from two 2,6-dimethylpyridine ligands. In the anion, the Au^{III} atom has a square-planar coordination geometry. The Au atoms each are located on an inversion center. In the cation, the Au—N bond length (Table 1) is in good agreement with the corresponding values in (X) and (XI) and in the anion, the Au—Cl bond lengths and angles (Table 1) are within a normal range, comparable with those in (II), (VIII) and (XII). In the crystal structure, intermolecular C—H...Cl hydrogen bonds are observed.

Experimental

A solution of 2,6-dimethylpyridine (0.12 g, 1.09 mmol) in methanol (15 ml) was added to a solution of HAuCl₃.3H₂O, (0.37 g, 1.09 mmol) in acetonitrile (15 ml). The resulting yellow solution was stirred for 10 min at 313 K, and then it was left to evaporate slowly at room temperature. After one week, yellow block crystals of (I) were isolated (yield 75.8%, 0.31 g; m. p. 489 K).

Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.96 (methyl) Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest residual electron density was found 0.90 Å from atom Au2 and the deepest hole 0.81 Å from atom Au2.

Figures

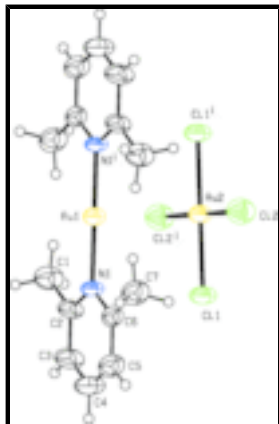


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level. [Symmetry code: (i) $-x, y, 1 - z$.]

Bis(2,6-dimethylpyridine- κ N)gold(I) tetrachloridoaurate(III)

Crystal data

[Au(C₇H₉N)₂][AuCl₄]

$M_r = 750.04$

Monoclinic, $C2/m$

Hall symbol: $-C 2y$

$a = 17.773 (3) \text{ \AA}$

$b = 6.8395 (8) \text{ \AA}$

$c = 8.3728 (14) \text{ \AA}$

$\beta = 110.929 (12)^\circ$

$V = 950.6 (3) \text{ \AA}^3$

$Z = 2$

$F_{000} = 684$

$D_x = 2.62 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 971 reflections

$\theta = 2.6\text{--}29.2^\circ$

$\mu = 15.97 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Block, yellow

$0.20 \times 0.12 \times 0.08 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.112$, $T_{\max} = 0.275$

5473 measured reflections

1384 independent reflections

1123 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.092$

$\theta_{\text{max}} = 29.2^\circ$

$\theta_{\text{min}} = 2.6^\circ$

$h = -23 \rightarrow 24$

$k = -9 \rightarrow 8$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 5.4887P]$$

$$R[F^2 > 2\sigma(F^2)] = 0.044$$

$$wR(F^2) = 0.115$$

$$S = 1.20$$

1384 reflections

69 parameters

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.004$$

$$\Delta\rho_{\max} = 1.76 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -2.1 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0	0.5	0.5	0.04157 (18)
Au2	0	0	0.5	0.0484 (2)
Cl1	0.13598 (17)	0	0.6416 (5)	0.0656 (9)
Cl2	0.0196 (2)	0	0.2445 (5)	0.0726 (10)
N1	0.1180 (5)	0.5	0.6531 (12)	0.044 (2)
C1	0.0754 (8)	0.5	0.8993 (16)	0.068 (4)
H1A	0.0803	0.6146	0.9684	0.081*
H1B	0.0238	0.5	0.8084	0.081*
C2	0.1398 (7)	0.5	0.8262 (15)	0.054 (3)
C3	0.2206 (8)	0.5	0.9317 (17)	0.071 (4)
H3	0.2353	0.5	1.05	0.085*
C4	0.2774 (8)	0.5	0.859 (2)	0.079 (5)
H4	0.3315	0.5	0.9288	0.095*
C5	0.2568 (8)	0.5	0.684 (2)	0.065 (3)
H5	0.2965	0.5	0.6361	0.078*
C6	0.1763 (6)	0.5	0.5816 (15)	0.047 (2)
C7	0.1497 (8)	0.5	0.3949 (19)	0.069 (4)
H7A	0.1702	0.386	0.3574	0.083*
H7B	0.0919	0.5	0.3473	0.083*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0319 (3)	0.0531 (4)	0.0374 (3)	0	0.00961 (19)	0
Au2	0.0327 (3)	0.0502 (4)	0.0538 (3)	0	0.0053 (2)	0
Cl1	0.0327 (12)	0.071 (2)	0.077 (2)	0	-0.0006 (12)	0
Cl2	0.0641 (19)	0.090 (3)	0.0611 (18)	0	0.0195 (15)	0
N1	0.024 (3)	0.050 (5)	0.050 (5)	0	0.002 (3)	0
C1	0.060 (7)	0.097 (12)	0.045 (6)	0	0.017 (5)	0
C2	0.038 (5)	0.065 (8)	0.042 (5)	0	-0.006 (4)	0

supplementary materials

C3	0.047 (6)	0.098 (12)	0.047 (6)	0	-0.008 (5)	0
C4	0.036 (6)	0.098 (13)	0.086 (10)	0	0.002 (6)	0
C5	0.045 (6)	0.075 (10)	0.078 (9)	0	0.026 (6)	0
C6	0.040 (5)	0.050 (6)	0.053 (6)	0	0.020 (4)	0
C7	0.057 (7)	0.088 (11)	0.074 (9)	0	0.037 (7)	0

Geometric parameters (Å, °)

Au1—N1	2.030 (8)	C2—C3	1.392 (15)
Au1—N1 ⁱ	2.030 (8)	C3—C4	1.35 (2)
Au2—Cl1 ⁱ	2.280 (3)	C3—H3	0.93
Au2—Cl1	2.280 (3)	C4—C5	1.38 (2)
Au2—Cl2	2.286 (4)	C4—H4	0.93
Au2—Cl2 ⁱ	2.286 (4)	C5—C6	1.381 (17)
N1—C2	1.360 (15)	C5—H5	0.93
N1—C6	1.370 (14)	C6—C7	1.463 (18)
C1—C2	1.479 (18)	C7—H7A	0.96
C1—H1A	0.96	C7—H7B	0.96
C1—H1B	0.96		
N1—Au1—N1 ⁱ	180.0 (3)	C4—C3—C2	118.8 (12)
Cl1 ⁱ —Au2—Cl1	180.00 (8)	C4—C3—H3	120.6
Cl1 ⁱ —Au2—Cl2	90.05 (14)	C2—C3—H3	120.6
Cl1—Au2—Cl2	89.95 (14)	C3—C4—C5	121.4 (12)
Cl1 ⁱ —Au2—Cl2 ⁱ	89.95 (14)	C3—C4—H4	119.3
Cl1—Au2—Cl2 ⁱ	90.05 (14)	C5—C4—H4	119.3
Cl2—Au2—Cl2 ⁱ	180.00 (17)	C4—C5—C6	119.0 (12)
C2—N1—C6	119.6 (9)	C4—C5—H5	120.5
C2—N1—Au1	120.7 (8)	C6—C5—H5	120.5
C6—N1—Au1	119.7 (7)	N1—C6—C5	120.3 (11)
C2—C1—H1A	109.5	N1—C6—C7	117.4 (10)
C2—C1—H1B	109.5	C5—C6—C7	122.3 (11)
H1A—C1—H1B	109.5	C6—C7—H7A	109.5
N1—C2—C3	120.9 (12)	C6—C7—H7B	109.5
N1—C2—C1	118.2 (10)	H7A—C7—H7B	109.5
C3—C2—C1	120.9 (11)		
C6—N1—C2—C3	0.000 (4)	C3—C4—C5—C6	0.000 (5)
Au1—N1—C2—C3	180.000 (4)	C2—N1—C6—C5	0.000 (4)
C6—N1—C2—C1	180.000 (4)	Au1—N1—C6—C5	180.000 (3)
Au1—N1—C2—C1	0.000 (3)	C2—N1—C6—C7	180.000 (3)
N1—C2—C3—C4	0.000 (6)	Au1—N1—C6—C7	0.000 (3)
C1—C2—C3—C4	180.000 (5)	C4—C5—C6—N1	0.000 (4)
C2—C3—C4—C5	0.000 (6)	C4—C5—C6—C7	180.000 (4)

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

Hydrogen-bond geometry (Å, °)

D—H \cdots A	D—H	H \cdots A	D \cdots A	D—H \cdots A
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