

Bis[dichlorido(5,5'-dimethyl-2,2'-bipyridine- κ^2N,N')gold(III)] tetrachloridoaurate(III) dichloridoaurate(I)

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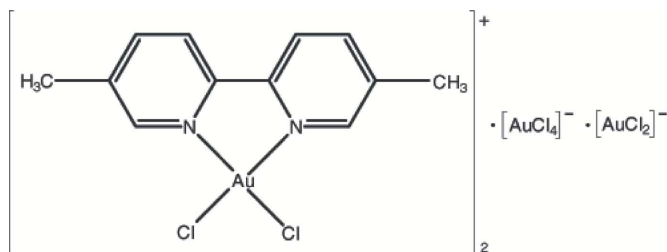
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.015$ Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 19.1.

The title compound, $[Au^{III}Cl_2(C_{12}H_{12}N_2)]_2[Au^{III}Cl_4][Au^I Cl_2]$, contains three distinct types of Au atom. In the cation, the Au^{III} atom is four-coordinated in a distorted square-planar arrangement by an N,N' -bidentate 5,5'-dimethyl-2,2'-bipyridine ligand and two terminal Cl atoms. In the $[AuCl_4]^-$ anion, the centrosymmetric Au^{III} atom has a square-planar coordination. The centrosymmetric $[AuCl_2]^-$ anion is linear. Intra- and intermolecular $C-H \cdots Cl$ hydrogen bonds help to establish the conformation and packing.

Related literature

For related structures, see: Abbate *et al.* (2000); Adams & Strähle (1982); Ahmadi, Amani & Khavasi (2008); Ahmadi, Dehghan, Amani & Khavasi (2008); Bjernemose *et al.* (2004); Hayoun *et al.* (2006); Hollis & Lippard (1983); McInnes *et al.* (1995); Yıldırım *et al.* (2008).



Experimental

Crystal data

$[AuCl_2(C_{12}H_{12}N_2)]_2[AuCl_4][AuCl_2]$ $a = 9.0698$ (4) Å
 $M_r = 1510.86$ $b = 10.0886$ (4) Å
 Triclinic, $P\bar{1}$ $c = 11.1678$ (5) Å

$\alpha = 91.155$ (4)°
 $\beta = 108.148$ (4)°
 $\gamma = 111.344$ (3)°
 $V = 894.09$ (7) Å³
 $Z = 1$

Mo $K\alpha$ radiation
 $\mu = 17.13$ mm⁻¹
 $T = 295$ K
 $0.41 \times 0.28 \times 0.08$ mm

Data collection

Stoe IPDS-2 diffractometer
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
 $T_{min} = 0.054$, $T_{max} = 0.341$

9898 measured reflections
 3651 independent reflections
 3193 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.059$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.112$
 $S = 1.05$
 3651 reflections

191 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.64$ e Å⁻³
 $\Delta\rho_{min} = -1.91$ e Å⁻³

Table 1
Selected bond lengths (Å).

| | | | |
|---------|-----------|---------|-----------|
| Au1—N1 | 2.028 (9) | Au2—Cl3 | 2.246 (5) |
| Au1—N2 | 2.027 (7) | Au2—Cl4 | 2.261 (3) |
| Au1—Cl1 | 2.252 (3) | Au3—Cl5 | 2.248 (3) |
| Au1—Cl2 | 2.262 (3) | | |

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

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------------------|-------|--------------|--------------|----------------|
| C1—H1 \cdots Cl1 | 0.93 | 2.59 | 3.203 (11) | 124 |
| C8—H8 \cdots Cl2 ⁱ | 0.93 | 2.75 | 3.666 (12) | 169 |
| C11—H11 \cdots Cl2 | 0.93 | 2.64 | 3.233 (11) | 122 |

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

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (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: HB2902).

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supplementary materials

Acta Cryst. (2009). E65, m335-m336 [doi:10.1107/S1600536809006436]

**Bis[dichlorido(5,5'-dimethyl-2,2'-bipyridine- κ^2N,N')gold(III)]
dichloridoaurate(I) tetrachloridoaurate(III)**

S. Karaca, M. Akkurt, N. Safari, V. Amani, O. Büyükgüngör and A. Abedi

Comment

Recently, we reported the synthesis and crystal structure of the $[\text{Au}(\text{dtbpy})\text{Cl}_2][\text{AuCl}_4]\cdot\text{CH}_3\text{CN}$, (II), (Yıldırım *et al.*, 2008) [where dtbpy is 4,4'-di-*tert*-butyl-2,2'-bipyridine]. There are several Au^{III} complexes, with formula, $[\text{AuCl}_2(\text{N}-\text{N})\text{X}]$, such as $[\text{AuCl}_2(\text{bipy})][\text{BF}_4]$, (III), (McInnes *et al.*, 1995), $[\text{AuCl}_2(\text{bipy})](\text{NO}_3)$, (IV), (Bjernemose *et al.*, 2004), $[\text{AuCl}_2(\text{bipy})][\text{AuBr}_4]$, (V), (Hayoun *et al.*, 2006), $[\text{AuCl}_2(\text{dmphen})][\text{AuCl}_4]$, (VI), (Ahmadi, Amani *et al.*, 2008) and $[\text{AuCl}_2(\text{phen})]\text{Cl}\cdot\text{H}_2\text{O}$, (VII), (Abbate *et al.*, 2000) [where bipy is 2,2'-bipyridine, dmphen is 4,7-diphenyl-1,10-phenanthroline and phen is 1,10-phenanthroline] have been synthesized and characterized by single-crystal X-ray diffraction methods. Two Au^{III} complexes with formula, $[\text{AuCl}_2\text{L}_2\text{X}]$, $[\text{AuCl}_2(\text{py})_2][\text{AuCl}_4]$, (VIII), and $[\text{AuCl}_2(\text{py})_2]\text{Cl}\cdot\text{H}_2\text{O}$, (IX), (Adams & Strähle 1982) [py is pyridine] and two mixed-valence $\text{Au}^{\text{I}}-\text{Au}^{\text{III}}$ complexes, $[\text{Au}(\text{terpy})\text{Cl}]_2[\text{AuCl}_2]_3[\text{AuCl}_4]$, (X), (Hollis & Lippard, 1983) and $[\text{Au}(\text{dmpy})_2][\text{AuCl}_4]$, (XI), (Ahmadi, Dehghan *et al.*, 2008) [where terpy is 2,2',2''-terpyridine and dmpy is 2,6-dimethylpyridine] 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 asymmetric unit of the title compound (I), (Fig. 1), there are one cation and two half-anions. In the cation, the Au^{III} atom is four-coordinated in a distorted square-planar configuration by two N atoms from the ligand and two terminal Cl atoms. In the anion AuCl_4 , the Au^{III} atom has a square-planar coordination. The anion AuCl_2 is linear. In the cation, the Au—Cl and Au—N bond lengths and angles (Table 1) are in good agreement with the corresponding values in (II), (III), (IV), (V), (VI), (VII), (VIII), (IX), (X) and (XI). In the anion, the Au—Cl bond lengths and angles (Table 1) are normal.

Intra and intermolecular C—H \cdots Cl hydrogen bonding interactions (Table 2) stabilize the molecular conformation and the packing arrangement (Fig. 2).

Experimental

A solution of 5,5'-dimethyl-2,2'-bipyridine (0.20 g, 1.09 mmol) in ethanol (20 ml) was added to a solution of $\text{HAuCl}_4\cdot 3\text{H}_2\text{O}$, (0.37 g, 1.09 mmol) in acetonitrile (20 ml) and the resulting yellow solution was stirred for 10 min at 313 K. Then, it was left to evaporate slowly at room temperature. After one week, yellow prismatic crystals of (I) were isolated (yield 0.28 g, 72.8%; m.p. 553 K).

Refinement

All H-atoms were placed in calculated positions with C—H = 0.93 Å and C—H 0.96 Å, and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{ring C})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl C})$. In the final Fourier map, the highest and deepest peaks were located 0.91 and 0.81 Å from atom Au1, respectively.

Figures

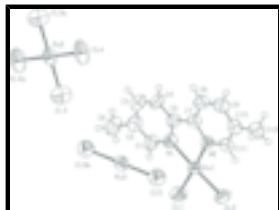


Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids for the non-hydrogen atoms. Symmetry code suffixes: (a) $-x, -y, -z$; (b) $2-x, 1-y, 1-z$.

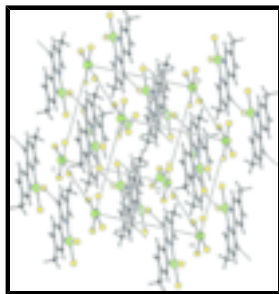


Fig. 2. A general view of the packing and hydrogen bonding interactions in (I).

Bis[dichlorido(5,5'-dimethyl-2,2'-bipyridine- κ^2N,N')gold(III)] tetrachloridoaurate(III) dichloridoaurate(I)

Crystal data

$[\text{AuCl}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)]_2[\text{AuCl}_4][\text{AuCl}_2]$

$M_r = 1510.86$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.0698\ (4)\ \text{\AA}$

$b = 10.0886\ (4)\ \text{\AA}$

$c = 11.1678\ (5)\ \text{\AA}$

$\alpha = 91.155\ (4)^\circ$

$\beta = 108.148\ (4)^\circ$

$\gamma = 111.344\ (3)^\circ$

$V = 894.09\ (7)\ \text{\AA}^3$

$Z = 1$

$F_{000} = 682$

$D_x = 2.806\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Cell parameters from 16778 reflections

$\theta = 1.9\text{--}28.0^\circ$

$\mu = 17.13\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Prism, yellow

$0.41 \times 0.28 \times 0.08\ \text{mm}$

Data collection

Stoe IPDS-2
diffractometer

Monochromator: plane graphite

Detector resolution: $6.67\ \text{pixels mm}^{-1}$

$T = 295\ \text{K}$

ω scans

Absorption correction: integration
(X-RED32; Stoe & Cie, 2002)

$T_{\min} = 0.054, T_{\max} = 0.341$

9898 measured reflections

3651 independent reflections

3193 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

$\theta_{\text{max}} = 26.5^\circ$

$\theta_{\text{min}} = 1.9^\circ$

$h = -10 \rightarrow 11$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

Refinement

| | |
|--|---|
| Refinement on F^2 | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | $w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.309P]$ |
| $wR(F^2) = 0.112$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{\max} = 0.001$ |
| 3651 reflections | $\Delta\rho_{\max} = 1.64 \text{ e } \text{\AA}^{-3}$ |
| 191 parameters | $\Delta\rho_{\min} = -1.91 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1+0.001XF_c^2\Lambda^3/\sin(2\theta)]^{-1/4}$ |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0.0042 (5) |

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| Au1 | 1.23403 (3) | 0.77774 (3) | 0.26312 (3) | 0.0544 (1) |
| Cl1 | 1.2859 (3) | 0.5914 (3) | 0.1987 (3) | 0.0790 (9) |
| Cl2 | 1.5117 (3) | 0.9173 (3) | 0.3196 (3) | 0.0782 (9) |
| N1 | 0.9831 (9) | 0.6658 (8) | 0.2201 (7) | 0.060 (2) |
| N2 | 1.1693 (8) | 0.9371 (7) | 0.3140 (6) | 0.0528 (19) |
| C1 | 0.9039 (11) | 0.5243 (9) | 0.1758 (9) | 0.066 (3) |
| C2 | 0.7317 (12) | 0.4506 (10) | 0.1500 (9) | 0.069 (3) |
| C3 | 0.6467 (11) | 0.5303 (11) | 0.1758 (10) | 0.076 (3) |
| C4 | 0.7298 (11) | 0.6737 (11) | 0.2244 (10) | 0.074 (3) |
| C5 | 0.8990 (11) | 0.7414 (9) | 0.2443 (8) | 0.060 (3) |
| C6 | 0.6455 (15) | 0.2922 (11) | 0.1035 (13) | 0.093 (4) |
| C7 | 1.0005 (10) | 0.8939 (9) | 0.2956 (8) | 0.056 (3) |
| C8 | 0.9407 (12) | 0.9933 (11) | 0.3240 (10) | 0.069 (3) |
| C9 | 1.0501 (13) | 1.1320 (11) | 0.3714 (11) | 0.076 (3) |
| C10 | 1.2194 (13) | 1.1753 (9) | 0.3894 (10) | 0.070 (3) |
| C11 | 1.2737 (11) | 1.0742 (9) | 0.3607 (8) | 0.060 (3) |

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| | | | | |
|------|-------------|-------------|-------------|-------------|
| C12 | 1.3426 (14) | 1.3307 (10) | 0.4439 (12) | 0.082 (4) |
| Au2 | 0.00000 | 0.00000 | 0.00000 | 0.0681 (2) |
| Cl3 | 0.2497 (5) | -0.0056 (5) | 0.0129 (5) | 0.1187 (16) |
| Cl4 | 0.1272 (6) | 0.2391 (3) | 0.0717 (3) | 0.1093 (12) |
| Au3 | 1.00000 | 0.50000 | 0.50000 | 0.0654 (2) |
| Cl5 | 1.2288 (4) | 0.7061 (3) | 0.5439 (3) | 0.0836 (7)* |
| H1 | 0.96620 | 0.47370 | 0.16190 | 0.0790* |
| H3 | 0.53150 | 0.48610 | 0.16010 | 0.0910* |
| H4 | 0.67160 | 0.72540 | 0.24380 | 0.0880* |
| H6A | 0.62170 | 0.24230 | 0.17190 | 0.1400* |
| H6B | 0.71750 | 0.25990 | 0.07430 | 0.1400* |
| H6C | 0.54210 | 0.27280 | 0.03460 | 0.1400* |
| H8 | 0.82660 | 0.96600 | 0.31100 | 0.0820* |
| H9 | 1.00990 | 1.19880 | 0.39200 | 0.0910* |
| H11 | 1.38780 | 1.10100 | 0.37400 | 0.0730* |
| H12A | 1.38440 | 1.34120 | 0.53520 | 0.1240* |
| H12B | 1.28570 | 1.39460 | 0.41790 | 0.1240* |
| H12C | 1.43510 | 1.35400 | 0.41270 | 0.1240* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| Au1 | 0.0476 (2) | 0.0555 (2) | 0.0651 (2) | 0.0246 (1) | 0.0206 (1) | 0.0069 (1) |
| Cl1 | 0.0748 (14) | 0.0681 (12) | 0.1089 (19) | 0.0387 (10) | 0.0390 (13) | 0.0006 (12) |
| Cl2 | 0.0476 (10) | 0.0728 (13) | 0.113 (2) | 0.0220 (9) | 0.0284 (11) | 0.0031 (13) |
| N1 | 0.053 (3) | 0.062 (4) | 0.059 (4) | 0.019 (3) | 0.017 (3) | 0.002 (3) |
| N2 | 0.051 (3) | 0.060 (3) | 0.053 (4) | 0.025 (3) | 0.021 (3) | 0.009 (3) |
| C1 | 0.062 (5) | 0.057 (4) | 0.074 (6) | 0.015 (4) | 0.027 (4) | 0.002 (4) |
| C2 | 0.067 (5) | 0.066 (5) | 0.062 (5) | 0.015 (4) | 0.022 (4) | 0.000 (4) |
| C3 | 0.051 (5) | 0.080 (6) | 0.079 (6) | 0.007 (4) | 0.023 (4) | 0.003 (5) |
| C4 | 0.043 (4) | 0.072 (5) | 0.091 (7) | 0.007 (4) | 0.021 (4) | 0.005 (5) |
| C5 | 0.057 (4) | 0.066 (5) | 0.061 (5) | 0.025 (4) | 0.025 (4) | 0.011 (4) |
| C6 | 0.077 (7) | 0.072 (6) | 0.107 (9) | 0.005 (5) | 0.031 (6) | -0.010 (6) |
| C7 | 0.050 (4) | 0.062 (4) | 0.060 (5) | 0.028 (3) | 0.018 (3) | 0.006 (4) |
| C8 | 0.061 (5) | 0.078 (5) | 0.079 (6) | 0.036 (4) | 0.030 (4) | 0.012 (5) |
| C9 | 0.085 (6) | 0.071 (5) | 0.094 (7) | 0.047 (5) | 0.040 (5) | 0.009 (5) |
| C10 | 0.084 (6) | 0.054 (4) | 0.071 (6) | 0.027 (4) | 0.026 (5) | 0.011 (4) |
| C11 | 0.060 (5) | 0.060 (4) | 0.062 (5) | 0.031 (4) | 0.014 (4) | 0.006 (4) |
| C12 | 0.087 (7) | 0.057 (5) | 0.103 (8) | 0.031 (4) | 0.029 (6) | 0.007 (5) |
| Au2 | 0.0810 (3) | 0.0527 (3) | 0.0547 (3) | 0.0170 (2) | 0.0130 (2) | 0.0067 (2) |
| Cl3 | 0.098 (2) | 0.133 (3) | 0.127 (3) | 0.052 (2) | 0.033 (2) | 0.018 (2) |
| Cl4 | 0.160 (3) | 0.0549 (12) | 0.0797 (18) | 0.0144 (15) | 0.0305 (19) | 0.0013 (11) |
| Au3 | 0.0724 (3) | 0.0670 (3) | 0.0672 (3) | 0.0335 (2) | 0.0296 (2) | 0.0161 (2) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------|-----------|-------|------------|
| Au1—N1 | 2.028 (9) | C5—C7 | 1.466 (12) |
| Au1—N2 | 2.027 (7) | C7—C8 | 1.375 (15) |
| Au1—Cl1 | 2.252 (3) | C8—C9 | 1.362 (15) |

| | | | |
|---------------------------|------------|--------------------------|------------|
| Au1—C12 | 2.262 (3) | C9—C10 | 1.380 (18) |
| Au2—C14 ⁱ | 2.261 (3) | C10—C11 | 1.355 (15) |
| Au2—C13 ⁱ | 2.246 (5) | C10—C12 | 1.530 (14) |
| Au2—C13 | 2.246 (5) | C1—H1 | 0.9300 |
| Au2—C14 | 2.261 (3) | C3—H3 | 0.9300 |
| Au3—C15 ⁱⁱ | 2.248 (3) | C4—H4 | 0.9300 |
| Au3—C15 | 2.248 (3) | C6—H6B | 0.9600 |
| N1—C1 | 1.343 (12) | C6—H6A | 0.9600 |
| N1—C5 | 1.334 (13) | C6—H6C | 0.9600 |
| N2—C7 | 1.375 (13) | C8—H8 | 0.9300 |
| N2—C11 | 1.339 (11) | C9—H9 | 0.9300 |
| C1—C2 | 1.393 (15) | C11—H11 | 0.9300 |
| C2—C3 | 1.380 (16) | C12—H12C | 0.9600 |
| C2—C6 | 1.496 (14) | C12—H12A | 0.9600 |
| C3—C4 | 1.369 (15) | C12—H12B | 0.9600 |
| C4—C5 | 1.375 (15) | | |
| Au1...C13 ⁱⁱⁱ | 3.588 (5) | N1...C7 | 2.368 (12) |
| Au1...C15 | 3.243 (3) | N1...C11 | 3.173 (9) |
| Au2...C7 ^{iv} | 3.490 (8) | N2...C12 | 3.165 (9) |
| Au2...C7 ^v | 3.490 (8) | N2...N1 | 2.619 (10) |
| Au3...C1 | 3.486 (9) | N2...C5 | 2.396 (12) |
| Au3...C1 ⁱⁱ | 3.486 (9) | C1...Au3 | 3.486 (9) |
| C11...C14 ^{vi} | 3.394 (4) | C1...Au3 | 3.486 (9) |
| C11...N1 | 3.173 (9) | C3...C11 ^{viii} | 3.625 (12) |
| C11...C1 | 3.203 (11) | C5...C14 ^{iv} | 3.477 (9) |
| C11...C12 | 3.166 (4) | C6...C13 | 3.564 (14) |
| C11...C3 ^{vi} | 3.625 (12) | C7...Au2 ^{iv} | 3.490 (8) |
| C12...N2 | 3.165 (9) | C7...Au2 ⁱⁱⁱ | 3.490 (8) |
| C12...C11 | 3.233 (11) | C8...C13 ^{iv} | 3.644 (12) |
| C12...C11 | 3.166 (4) | C10...C14 ⁱⁱⁱ | 3.513 (11) |
| C12...C11 ^{vii} | 3.476 (9) | C11...C12 ^{vii} | 3.476 (9) |
| C12...C15 ^{vii} | 3.650 (4) | C12...C12 ^{xi} | 3.448 (15) |
| C13...C6 | 3.564 (14) | C4...H8 | 2.8100 |
| C13...C8 ^{iv} | 3.644 (12) | C8...H4 | 2.7900 |
| C13...C14 | 3.185 (7) | H1...C11 | 2.5900 |
| C13...Au1 ^v | 3.588 (5) | H1...H6B | 2.3900 |
| C13...C14 ⁱ | 3.188 (7) | H3...C11 ^{viii} | 2.9300 |
| C14...C13 ⁱ | 3.188 (7) | H3...H6C | 2.5900 |
| C14...C10 ^v | 3.513 (11) | H4...C8 | 2.7900 |
| C14...C5 ^{iv} | 3.477 (9) | H4...C11 ^{viii} | 3.1200 |
| C14...C13 | 3.185 (7) | H4...C12 ^{viii} | 3.0500 |
| C14...C11 ^{viii} | 3.394 (4) | H4...H8 | 2.2800 |
| C14...N1 ^{iv} | 3.367 (8) | H6A...C15 ⁱⁱ | 2.9900 |
| C15...Au1 | 3.243 (3) | H6B...H1 | 2.3900 |

supplementary materials

| | | | |
|--|------------|--------------------------|------------|
| Cl5...Cl2 ^{vii} | 3.650 (4) | H6B...Cl3 ^{ix} | 2.8700 |
| Cl1...H4 ^{vi} | 3.1200 | H6C...H3 | 2.5900 |
| Cl1...H1 | 2.5900 | H6C...Cl3 | 3.0200 |
| Cl1...H3 ^{vi} | 2.9300 | H8...H4 | 2.2800 |
| Cl2...H8 ^{vi} | 2.7500 | H8...C4 | 2.8100 |
| Cl2...H11 | 2.6400 | H8...Cl2 ^{viii} | 2.7500 |
| Cl2...H4 ^{vi} | 3.0500 | H9...H12B | 2.4800 |
| Cl3...H6C | 3.0200 | H9...Cl5 ^x | 2.9300 |
| Cl3...H6B ^{ix} | 2.8700 | H11...Cl2 | 2.6400 |
| Cl5...H11 ^{vii} | 3.1200 | H11...H12C | 2.4300 |
| Cl5...H6A ⁱⁱ | 2.9900 | H11...Cl5 ^{vii} | 3.1200 |
| Cl5...H9 ^x | 2.9300 | H12B...H9 | 2.4800 |
| N1...Cl4 ^{iv} | 3.367 (8) | H12C...H11 | 2.4300 |
| N1...N2 | 2.619 (10) | | |
| Cl1—Au1—Cl2 | 89.07 (11) | C7—C8—C9 | 119.4 (11) |
| Cl1—Au1—N1 | 95.5 (2) | C8—C9—C10 | 121.3 (11) |
| Cl1—Au1—N2 | 175.8 (2) | C11—C10—C12 | 121.1 (11) |
| Cl2—Au1—N1 | 175.3 (2) | C9—C10—C11 | 117.6 (9) |
| Cl2—Au1—N2 | 95.0 (2) | C9—C10—C12 | 121.3 (10) |
| N1—Au1—N2 | 80.5 (3) | N2—C11—C10 | 122.5 (10) |
| Cl3 ⁱ —Au2—Cl4 ⁱ | 89.95 (19) | C2—C1—H1 | 119.00 |
| Cl3—Au2—Cl4 ⁱ | 90.05 (19) | N1—C1—H1 | 119.00 |
| Cl3—Au2—Cl4 | 89.95 (19) | C2—C3—H3 | 120.00 |
| Cl3—Au2—Cl3 ⁱ | 180.00 | C4—C3—H3 | 120.00 |
| Cl3 ⁱ —Au2—Cl4 | 90.05 (19) | C3—C4—H4 | 120.00 |
| Cl4—Au2—Cl4 ⁱ | 180.00 | C5—C4—H4 | 120.00 |
| Cl5—Au3—Cl5 ⁱⁱ | 180.00 | C2—C6—H6A | 109.00 |
| Au1—N1—C1 | 124.0 (7) | C2—C6—H6B | 109.00 |
| Au1—N1—C5 | 115.3 (6) | C2—C6—H6C | 109.00 |
| C1—N1—C5 | 120.7 (9) | H6B—C6—H6C | 109.00 |
| Au1—N2—C11 | 126.2 (7) | H6A—C6—H6B | 109.00 |
| Au1—N2—C7 | 113.9 (5) | H6A—C6—H6C | 109.00 |
| C7—N2—C11 | 120.0 (8) | C7—C8—H8 | 120.00 |
| N1—C1—C2 | 122.3 (10) | C9—C8—H8 | 120.00 |
| C3—C2—C6 | 121.8 (11) | C10—C9—H9 | 119.00 |
| C1—C2—C3 | 116.3 (9) | C8—C9—H9 | 119.00 |
| C1—C2—C6 | 121.8 (10) | N2—C11—H11 | 119.00 |
| C2—C3—C4 | 120.9 (10) | C10—C11—H11 | 119.00 |
| C3—C4—C5 | 120.1 (10) | C10—C12—H12A | 110.00 |
| N1—C5—C4 | 119.7 (8) | C10—C12—H12B | 109.00 |
| N1—C5—C7 | 115.4 (9) | C10—C12—H12C | 109.00 |
| C4—C5—C7 | 124.8 (9) | H12A—C12—H12B | 109.00 |
| N2—C7—C5 | 115.0 (8) | H12A—C12—H12C | 109.00 |
| N2—C7—C8 | 119.3 (8) | H12B—C12—H12C | 109.00 |
| C5—C7—C8 | 125.8 (9) | | |

| | | | |
|----------------|------------|----------------|-------------|
| Cl1—Au1—N1—C1 | 3.4 (7) | C11—N2—C7—C8 | 0.9 (12) |
| N2—Au1—N1—C1 | -177.7 (8) | N1—C1—C2—C3 | -1.7 (14) |
| Cl1—Au1—N1—C5 | -179.5 (6) | N1—C1—C2—C6 | -178.6 (10) |
| N2—Au1—N1—C5 | -0.7 (6) | C6—C2—C3—C4 | 176.7 (10) |
| Cl2—Au1—N2—C7 | -179.0 (5) | C1—C2—C3—C4 | -0.2 (15) |
| N1—Au1—N2—C7 | 0.0 (6) | C2—C3—C4—C5 | 2.1 (16) |
| Cl2—Au1—N2—C11 | 1.5 (7) | C3—C4—C5—C7 | 180.0 (9) |
| N1—Au1—N2—C11 | -179.5 (7) | C3—C4—C5—N1 | -2.2 (14) |
| Au1—N1—C1—C2 | 178.6 (7) | C4—C5—C7—N2 | 176.7 (8) |
| C5—N1—C1—C2 | 1.7 (14) | C4—C5—C7—C8 | -4.2 (15) |
| Au1—N1—C5—C4 | -176.8 (7) | N1—C5—C7—N2 | -1.2 (11) |
| C1—N1—C5—C4 | 0.4 (13) | N1—C5—C7—C8 | 177.9 (9) |
| Au1—N1—C5—C7 | 1.2 (10) | C5—C7—C8—C9 | 180.0 (9) |
| C1—N1—C5—C7 | 178.4 (8) | N2—C7—C8—C9 | -0.9 (14) |
| Au1—N2—C11—C10 | 178.3 (7) | C7—C8—C9—C10 | 1.1 (16) |
| C7—N2—C11—C10 | -1.1 (13) | C8—C9—C10—C11 | -1.3 (16) |
| Au1—N2—C7—C8 | -178.6 (7) | C8—C9—C10—C12 | -179.4 (10) |
| Au1—N2—C7—C5 | 0.6 (9) | C12—C10—C11—N2 | 179.4 (9) |
| C11—N2—C7—C5 | -179.9 (7) | C9—C10—C11—N2 | 1.3 (14) |

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x+1, y+1, z$; (iv) $-x+1, -y+1, -z$; (v) $x-1, y-1, z$; (vi) $x+1, y, z$; (vii) $-x+3, -y+2, -z+1$; (viii) $x-1, y, z$; (ix) $-x+1, -y, -z$; (x) $-x+2, -y+2, -z+1$; (xi) $-x+3, -y+3, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C1—H1 \cdots C11 | 0.93 | 2.59 | 3.203 (11) | 124 |
| C8—H8 \cdots C12 ^{viii} | 0.93 | 2.75 | 3.666 (12) | 169 |
| C11—H11 \cdots C12 | 0.93 | 2.64 | 3.233 (11) | 122 |

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

Fig. 1

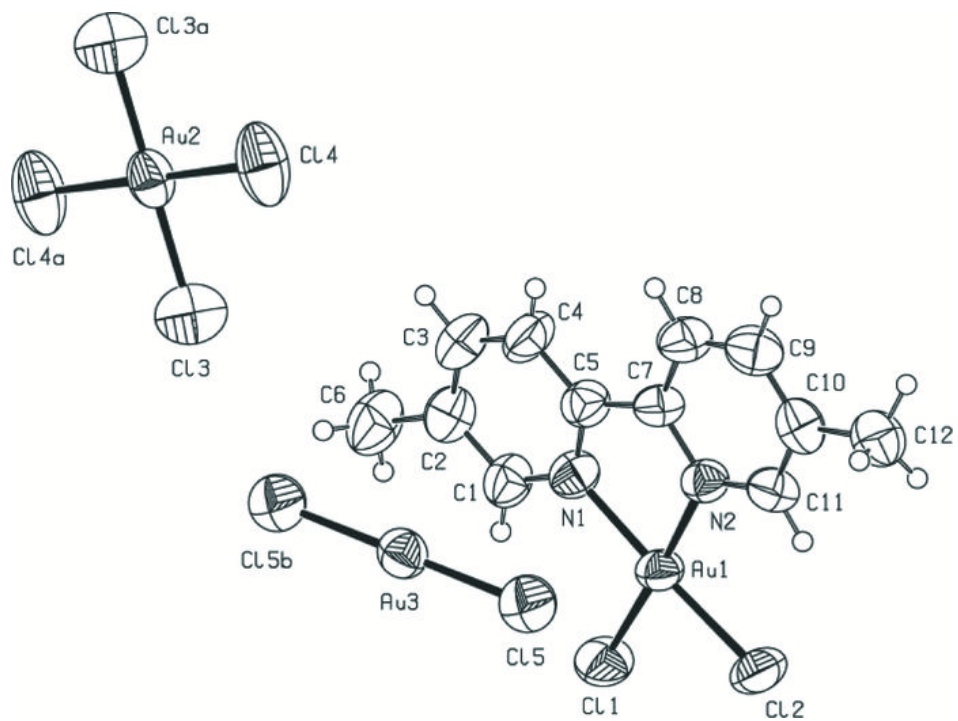


Fig. 2

