



# Crystal structure of chlorido(2-[[2-(phenylcarbamothioyl)hydrazin-1-ylidene](pyridin-2-yl)-methyl]pyridin-1-ium)gold(I) chloride sesquihydrate

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**Keywords:** crystal structure; gold(I) complex; thiosemicarbazone; hydrogen bonding

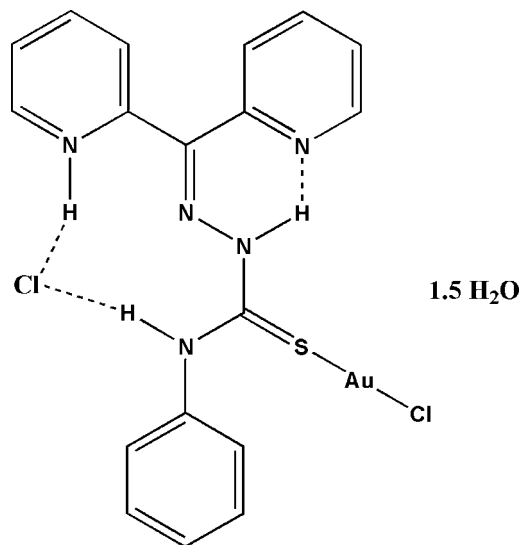
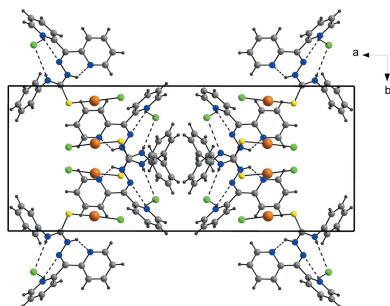
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The title complex,  $[\text{AuCl}(\text{C}_{18}\text{H}_{16}\text{N}_5\text{S})]\text{Cl}\cdot 1.5\text{H}_2\text{O}$ , may be considered as a gold(I) compound with the corresponding metal site coordinated by a thiosemicarbazone ligand through the S atom. The ligand adopts an *E* conformation and the gold(I) atom displays the expected linear geometry with a Cl atom also bonded to the metal ion  $[\text{Cl}-\text{Au}-\text{S} = 174.23(5)^\circ]$ . One of the pyridyl rings is protonated, giving the gold complex an overall positive charge. Two solvent water molecules, one of which is located on a twofold rotation axis, and a non-coordinating chloride ion complete the structural assembly. The molecular structure is stabilized by intramolecular and intermolecular  $\text{N}-\text{H}\cdots\text{Cl}$ ,  $\text{N}-\text{H}\cdots\text{N}$ ,  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonding.

## 1. Chemical context

Thiosemicarbazones are generated from reactions of thiosemicarbazides with either an aldehyde or a ketone. They are compounds that can coordinate to transition metals and exhibit keto–enol tautomerism (Duan *et al.*, 1996). Thiosemicarbazones are known to have diverse biological activity, including anti-malarial properties and antibacterial, anti-tubercular, antiviral and antitumor activity (Beraldo & Gambino, 2004, Casini *et al.*, 2008, Khanye *et al.*, 2010). The study of gold compounds with thiosemicarbazones has great importance: the literature reports that some compounds of this type have been shown to exhibit biological activity and have potential applications (Casini *et al.*, 2008, Lessa *et al.*, 2011).



**Table 1**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N5-H5A\cdots Cl2$	0.86	2.46	3.246 (4)	153
$N4-H4A\cdots N2$	0.86	1.97	2.629 (5)	133
$N1-H1A\cdots Cl2$	0.80 (4)	2.26 (4)	2.989 (4)	150 (4)
$O1-H1W1\cdots Cl1^i$	0.80 (2)	2.70 (5)	3.353 (4)	140 (6)
$O1-H1W2\cdots Cl2^{ii}$	0.81 (2)	2.39 (2)	3.206 (4)	177 (6)
$O2-H2W2\cdots O1$	0.82 (2)	2.06 (3)	2.855 (5)	163 (7)

Symmetry codes: (i)  $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$ ; (ii)  $x, -y + 1, z - \frac{1}{2}$ .

## 2. Structural commentary

In the title complex (Fig. 1), the di-2-pyridyl ketone phenylthiosemicarbazone ligand is protonated at the pyridine (py) nitrogen and only the sulfur donor atom is used to bond to the central metal ion. The thiosemicarbazone adopts the *E* conformation in relation to the  $C6=C3$  and  $N4-C12$  bonds.

The crystal structure data confirm reduction of gold(III) of the starting material  $[HPy][AuCl_4]$  during the synthesis. Two solvent water molecules and a non-coordinating chloride ion complete the structural assembly and are hydrogen bonded to the cationic complex.

The gold(I) atom displays the expected linear geometry, with a  $Cl-Au-S$  coordination angle of  $174.23(5)^\circ$ , close to the ideal angle of  $180^\circ$  expected for *sp* hybridization of the metal.

The  $C12-S1$  bond length reported for di-2-pyridyl ketone phenylthiosemicarbazone is  $1.676(2)$  Å and it is lengthened to  $1.713(4)$  Å on coordination to gold; this is typical of the ketone form with a concomitant shortening of the  $N3-N4$  bond (Suni *et al.*, 2006).

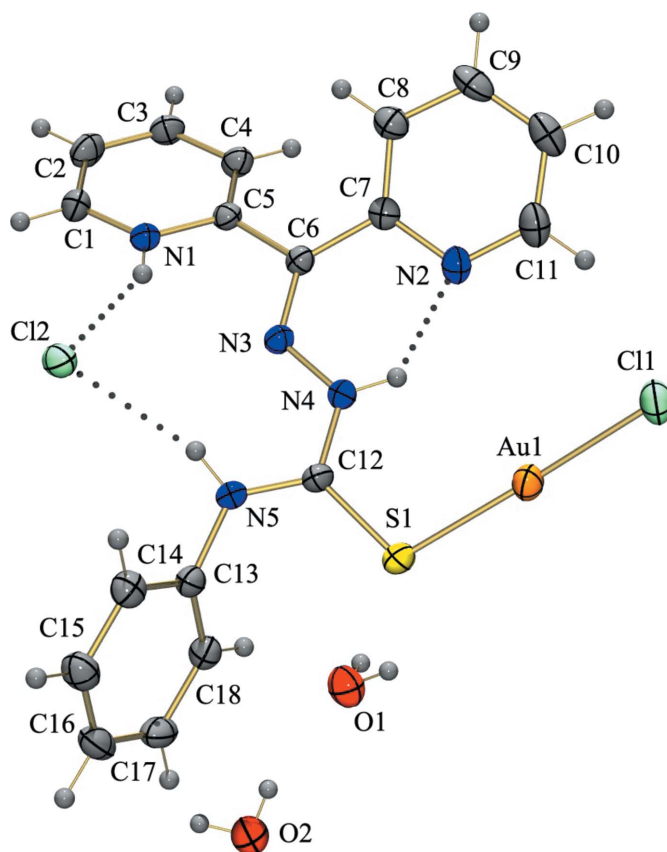
An intramolecular  $N4-H4A\cdots N2$  hydrogen bond (Table 1) is observed.

## 3. Supramolecular features

In the crystal, the chloride ion is linked to the complex molecule by  $N-H\cdots Cl$  hydrogen bonds. The molecular structure is also stabilized by intermolecular  $O-H\cdots Cl$  and  $O-H\cdots O$  hydrogen bonding involving the water molecules. Therefore, upon protonation of the ligand, hydrogen-bond formation with the chloride ion results in a stabilization of the conformation of the cationic gold complex, and hydrogen bonding plays an important role in the crystallization of the compound (Table 1 and Fig. 2).

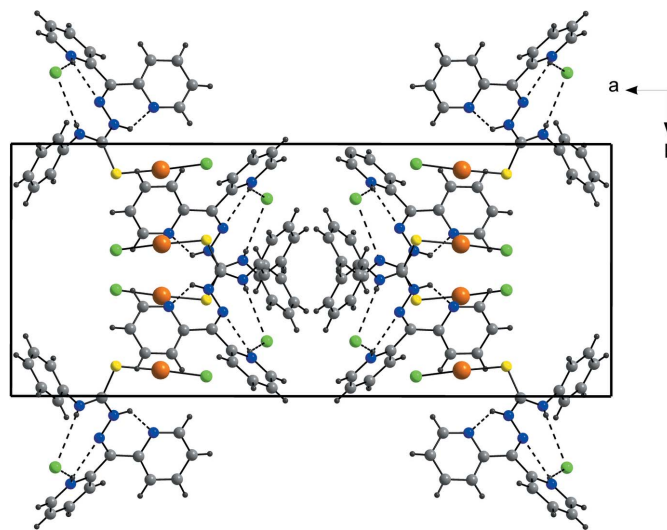
## 4. Related studies

For the preparation of coordination compounds of thiosemicarbazones with gold, see: Castiñeiras *et al.* (2012); Khanye *et al.* (2010); Lessa *et al.* (2011); Sreekanth *et al.* (2004). For the spectroscopic (FT-IR) properties of thiosemicarbazones and the crystal structure of thiosemicarbazones, see: Beraldo & Gambino (2004); Duan *et al.* (1996); Pereiras-Gabián *et al.* (2004); Suni *et al.* (2006). For the



**Figure 1**  
Perspective view of  $[AuCl(C_{18}H_{16}N_5S)]Cl \cdot 1.5H_2O$  with 30% probability ellipsoids and atom labeling.

crystal structures of di-2-pyridyl ketone phenylthiosemicarbazone and coordination compounds with this thiosemicarbazone, see: Bernhardt *et al.* (2009); Philip *et al.* (2005); Suni *et al.* (2006, 2007). For structure-activity studies of



**Figure 2**  
Perspective view of the compound showing the components connected by  $N-H\cdots Cl$  and  $N-H\cdots N$  hydrogen bonds (dashed lines), viewed along the *c* axis. Solvent water molecules have been omitted for clarity.

thiosemicarbazones, see: Bernhardt *et al.* (2009); Casini *et al.* (2008); Duan *et al.* (1996).

### 5. Synthesis and crystallization

Di-2-pyridyl ketone phenylthiosemicarbazone (1 mmol) was dissolved in about 5 ml of CH<sub>3</sub>CN and added to a solution of [HPy][AuCl<sub>4</sub>] (1 mmol) in 5 ml of CH<sub>3</sub>CN. A clear yellow solution was formed after heating the mixture to reflux for three h. Orange crystals deposited upon slow cooling of the solvent. Yield: 69%, m.p. 491 K. Elemental analysis, found: C, 33.71; H, 3.15; N, 10.04%; calculated for C<sub>36</sub>H<sub>38</sub>Au<sub>2</sub>Cl<sub>4</sub>N<sub>10</sub>O<sub>3</sub>S<sub>2</sub>: C, 33.87; H, 3.16; N, 10.97%. IR ( $\nu_{\max}$  cm<sup>-1</sup>): 3421 (O–H), 3281 (N–H), 2927 (N–H<sup>+</sup>), 1694 (C=N), 1150 (N–N), 765 (C=S).

### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms potentially involved in hydrogen-bonding interactions were located in difference electron-density maps and their positional and isotropic displacement parameters were refined. Hydrogen atoms of water molecules were refined with distance restraints, with an H...H separation of 1.38 (2) Å, the H–O distance restrained to 0.82 (2) Å and with  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{O})$ . Other H atoms were included in the refinement at calculated positions and treated as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Acknowledgements

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**Table 2**  
Experimental details.

Crystal data	
Chemical formula	[AuCl(C <sub>18</sub> H <sub>16</sub> N <sub>5</sub> S)]Cl·1.5H <sub>2</sub> O
$M_r$	629.31
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	296
$a, b, c$ (Å)	31.0939 (7), 12.2704 (3), 11.8851 (3)
$\beta$ (°)	110.174 (1)
$V$ (Å <sup>3</sup> )	4256.38 (18)
$Z$	8
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	7.28
Crystal size (mm)	0.24 × 0.22 × 0.14
Data collection	
Diffractometer	Bruker CCD SMART APEXII
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2009)
$T_{\min}, T_{\max}$	0.274, 0.429
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	15424, 4345, 3220
$R_{\text{int}}$	0.038
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.072, 0.97
No. of reflections	4345
No. of parameters	271
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.97, -0.78

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Crystal Impact, 2014) and *publCIF* (Westrip, 2010).

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## supporting information

*Acta Cryst.* (2015). E71, 1070-1072 [https://doi.org/10.1107/S2056989015015480]

## Crystal structure of chlorido(2-[[2-(phenylcarbamothioyl)hydrazin-1-ylidene]pyridin-2-yl)methyl]pyridin-1-ium)gold(I) chloride sesquihydrate

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### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Crystal Impact, 2014); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

### Chlorido(2-[[2-(phenylcarbamothioyl)hydrazin-1-ylidene]pyridin-2-yl)methyl]pyridin-1-ium)gold(I) chloride sesquihydrate

#### Crystal data

[AuCl(C<sub>18</sub>H<sub>16</sub>N<sub>5</sub>S)]Cl·1.5H<sub>2</sub>O

$M_r = 629.31$

Monoclinic, *C2/c*

$a = 31.0939$  (7) Å

$b = 12.2704$  (3) Å

$c = 11.8851$  (3) Å

$\beta = 110.174$  (1)°

$V = 4256.38$  (18) Å<sup>3</sup>

$Z = 8$

$F(000) = 2424$

$D_x = 1.964$  Mg m<sup>-3</sup>

Melting point: 491 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4811 reflections

$\theta = 2.7\text{--}25.2^\circ$

$\mu = 7.28$  mm<sup>-1</sup>

$T = 296$  K

Block, red

0.24 × 0.22 × 0.14 mm

#### Data collection

Bruker CCD SMART APEXII  
diffractometer

Radiation source: fine-focus sealed tube

$\phi$  &  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2009)

$T_{\min} = 0.274$ ,  $T_{\max} = 0.429$

15424 measured reflections

4345 independent reflections

3220 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 26.4^\circ$ ,  $\theta_{\min} = 1.8^\circ$

$h = -37\text{--}38$

$k = -14\text{--}15$

$l = -14\text{--}14$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.072$

$S = 0.97$

4345 reflections

271 parameters

3 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.97 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.78 \text{ e } \text{\AA}^{-3}$$

### 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 ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.25092 (2)	0.60284 (2)	0.04569 (2)	0.04892 (9)
S1	0.32514 (5)	0.61867 (10)	0.16165 (13)	0.0581 (4)
Cl1	0.17486 (5)	0.57863 (11)	-0.05533 (12)	0.0610 (4)
C12	0.34886 (15)	0.4928 (3)	0.1607 (4)	0.0388 (10)
N3	0.35315 (13)	0.3345 (3)	0.0578 (3)	0.0370 (9)
N5	0.38617 (12)	0.4607 (3)	0.2458 (3)	0.0424 (9)
H5A	0.3953	0.3954	0.2403	0.051*
N4	0.32925 (13)	0.4234 (3)	0.0690 (3)	0.0401 (9)
H4A	0.3022	0.4355	0.0190	0.048*
C13	0.41343 (15)	0.5235 (4)	0.3473 (4)	0.0410 (11)
C5	0.36773 (15)	0.1810 (3)	-0.0344 (4)	0.0355 (10)
C6	0.33459 (15)	0.2653 (3)	-0.0268 (3)	0.0342 (10)
C7	0.28703 (16)	0.2612 (3)	-0.1109 (3)	0.0376 (10)
C4	0.36887 (17)	0.1356 (3)	-0.1392 (4)	0.0431 (11)
H4	0.3469	0.1549	-0.2121	0.052*
C1	0.43375 (18)	0.0813 (3)	0.0737 (5)	0.0479 (12)
H1	0.4560	0.0642	0.1470	0.057*
C18	0.43406 (17)	0.6200 (4)	0.3336 (5)	0.0472 (12)
H18	0.4292	0.6490	0.2579	0.057*
C15	0.45009 (18)	0.5339 (4)	0.5600 (4)	0.0560 (14)
H15	0.4557	0.5049	0.6360	0.067*
C16	0.47070 (18)	0.6300 (4)	0.5471 (5)	0.0585 (14)
H16	0.4903	0.6657	0.6142	0.070*
C14	0.42124 (16)	0.4803 (4)	0.4608 (4)	0.0481 (12)
H14	0.4071	0.4158	0.4697	0.058*
C17	0.46232 (17)	0.6725 (4)	0.4362 (5)	0.0553 (13)
H17	0.4758	0.7384	0.4286	0.066*
C3	0.40278 (18)	0.0613 (4)	-0.1356 (4)	0.0492 (12)
H3	0.4037	0.0304	-0.2062	0.059*
C2	0.43484 (18)	0.0335 (4)	-0.0286 (5)	0.0536 (13)
H2	0.4573	-0.0177	-0.0254	0.064*
N2	0.26250 (14)	0.3552 (3)	-0.1220 (3)	0.0471 (10)
N1	0.40084 (13)	0.1526 (3)	0.0690 (3)	0.0393 (9)
C9	0.22292 (19)	0.1715 (5)	-0.2508 (5)	0.0588 (14)
H9	0.2095	0.1095	-0.2936	0.071*
C8	0.26759 (17)	0.1682 (4)	-0.1724 (4)	0.0486 (12)

H8	0.2844	0.1038	-0.1612	0.058*
C11	0.21949 (19)	0.3548 (5)	-0.1966 (4)	0.0586 (14)
H11	0.2024	0.4181	-0.2030	0.070*
C10	0.19855 (19)	0.2663 (5)	-0.2653 (4)	0.0592 (14)
H10	0.1688	0.2710	-0.3197	0.071*
C12	0.42609 (4)	0.21756 (9)	0.32609 (9)	0.0506 (3)
O1	0.42303 (14)	0.7870 (4)	0.0930 (3)	0.0663 (10)
H1W1	0.3956 (7)	0.787 (6)	0.069 (6)	0.099*
H1W2	0.424 (2)	0.783 (5)	0.025 (3)	0.099*
O2	0.5000	0.9028 (5)	0.2500	0.087 (2)
H2W2	0.4803 (19)	0.859 (4)	0.213 (6)	0.130*
H1A	0.3997 (14)	0.186 (3)	0.126 (4)	0.033 (13)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Au1	0.04494 (14)	0.05060 (13)	0.04726 (13)	0.01206 (9)	0.01084 (10)	-0.00251 (9)
S1	0.0458 (8)	0.0439 (7)	0.0735 (9)	0.0109 (6)	0.0064 (7)	-0.0198 (6)
Cl1	0.0451 (8)	0.0752 (9)	0.0550 (8)	0.0134 (6)	0.0075 (7)	0.0022 (6)
C12	0.042 (3)	0.032 (2)	0.043 (2)	0.001 (2)	0.014 (2)	-0.005 (2)
N3	0.041 (2)	0.033 (2)	0.0358 (19)	0.0044 (16)	0.0122 (18)	-0.0029 (16)
N5	0.043 (3)	0.0311 (19)	0.047 (2)	0.0033 (16)	0.008 (2)	-0.0065 (17)
N4	0.033 (2)	0.037 (2)	0.046 (2)	0.0049 (16)	0.0089 (19)	-0.0062 (17)
C13	0.036 (3)	0.038 (2)	0.047 (3)	0.004 (2)	0.012 (2)	-0.004 (2)
C5	0.040 (3)	0.030 (2)	0.036 (2)	-0.0010 (19)	0.012 (2)	0.0018 (19)
C6	0.038 (3)	0.033 (2)	0.033 (2)	0.0017 (18)	0.013 (2)	0.0008 (19)
C7	0.041 (3)	0.042 (2)	0.032 (2)	0.000 (2)	0.016 (2)	0.002 (2)
C4	0.052 (3)	0.040 (2)	0.037 (2)	0.005 (2)	0.015 (2)	-0.002 (2)
C1	0.050 (3)	0.040 (3)	0.047 (3)	0.008 (2)	0.007 (3)	0.003 (2)
C18	0.046 (3)	0.043 (3)	0.050 (3)	0.004 (2)	0.014 (3)	0.003 (2)
C15	0.056 (4)	0.066 (3)	0.044 (3)	0.002 (3)	0.015 (3)	-0.008 (3)
C16	0.040 (3)	0.066 (3)	0.060 (3)	0.000 (3)	0.006 (3)	-0.023 (3)
C14	0.045 (3)	0.050 (3)	0.052 (3)	0.000 (2)	0.019 (3)	0.001 (2)
C17	0.046 (3)	0.041 (3)	0.075 (4)	-0.005 (2)	0.016 (3)	-0.012 (3)
C3	0.056 (3)	0.043 (3)	0.050 (3)	0.003 (2)	0.020 (3)	-0.012 (2)
C2	0.053 (3)	0.044 (3)	0.069 (4)	0.011 (2)	0.027 (3)	-0.003 (3)
N2	0.043 (3)	0.054 (2)	0.040 (2)	0.0091 (19)	0.008 (2)	0.0055 (18)
N1	0.044 (3)	0.033 (2)	0.037 (2)	0.0027 (17)	0.010 (2)	-0.0038 (18)
C9	0.045 (3)	0.073 (4)	0.054 (3)	-0.024 (3)	0.012 (3)	-0.006 (3)
C8	0.045 (3)	0.050 (3)	0.051 (3)	-0.006 (2)	0.016 (3)	-0.001 (2)
C11	0.048 (4)	0.076 (4)	0.047 (3)	0.013 (3)	0.009 (3)	0.008 (3)
C10	0.041 (3)	0.088 (4)	0.044 (3)	-0.006 (3)	0.009 (3)	-0.001 (3)
Cl2	0.0610 (9)	0.0450 (6)	0.0386 (6)	-0.0022 (6)	0.0080 (6)	0.0000 (5)
O1	0.065 (3)	0.079 (2)	0.051 (2)	0.002 (2)	0.015 (2)	0.003 (2)
O2	0.077 (5)	0.064 (4)	0.092 (5)	0.000	-0.004 (4)	0.000



*Geometric parameters (Å, °)*

Au1—S1	2.2515 (14)	C18—H18	0.9300
Au1—C11	2.2725 (14)	C15—C16	1.376 (7)
S1—C12	1.713 (4)	C15—C14	1.377 (6)
C12—N5	1.309 (5)	C15—H15	0.9300
C12—N4	1.351 (5)	C16—C17	1.357 (7)
N3—C6	1.290 (5)	C16—H16	0.9300
N3—N4	1.353 (5)	C14—H14	0.9300
N5—C13	1.436 (5)	C17—H17	0.9300
N5—H5A	0.8600	C3—C2	1.362 (7)
N4—H4A	0.8600	C3—H3	0.9300
C13—C18	1.383 (6)	C2—H2	0.9300
C13—C14	1.391 (6)	N2—C11	1.325 (6)
C5—N1	1.349 (5)	N1—H1A	0.80 (4)
C5—C4	1.375 (6)	C9—C10	1.366 (7)
C5—C6	1.485 (6)	C9—C8	1.381 (7)
C6—C7	1.473 (6)	C9—H9	0.9300
C7—N2	1.364 (5)	C8—H8	0.9300
C7—C8	1.378 (6)	C11—C10	1.380 (7)
C4—C3	1.384 (6)	C11—H11	0.9300
C4—H4	0.9300	C10—H10	0.9300
C1—N1	1.332 (6)	O1—H1W1	0.80 (2)
C1—C2	1.361 (7)	O1—H1W2	0.813 (19)
C1—H1	0.9300	O2—H2W2	0.82 (2)
C18—C17	1.390 (6)		
S1—Au1—C11	174.23 (5)	C16—C15—H15	119.9
C12—S1—Au1	105.72 (16)	C14—C15—H15	119.9
N5—C12—N4	117.8 (4)	C17—C16—C15	119.8 (5)
N5—C12—S1	122.3 (3)	C17—C16—H16	120.1
N4—C12—S1	119.8 (3)	C15—C16—H16	120.1
C6—N3—N4	119.6 (4)	C15—C14—C13	119.5 (5)
C12—N5—C13	126.6 (4)	C15—C14—H14	120.2
C12—N5—H5A	116.7	C13—C14—H14	120.2
C13—N5—H5A	116.7	C16—C17—C18	121.7 (5)
C12—N4—N3	118.5 (4)	C16—C17—H17	119.2
C12—N4—H4A	120.7	C18—C17—H17	119.2
N3—N4—H4A	120.7	C2—C3—C4	119.9 (5)
C18—C13—C14	120.5 (4)	C2—C3—H3	120.1
C18—C13—N5	121.6 (4)	C4—C3—H3	120.1
C14—C13—N5	117.7 (4)	C1—C2—C3	119.4 (5)
N1—C5—C4	118.1 (4)	C1—C2—H2	120.3
N1—C5—C6	116.9 (4)	C3—C2—H2	120.3
C4—C5—C6	124.9 (4)	C11—N2—C7	117.6 (4)
N3—C6—C7	128.7 (4)	C1—N1—C5	122.8 (4)
N3—C6—C5	111.9 (4)	C1—N1—H1A	124 (3)
C7—C6—C5	119.4 (4)	C5—N1—H1A	113 (3)

N2—C7—C8	121.4 (4)	C10—C9—C8	119.7 (5)
N2—C7—C6	115.7 (4)	C10—C9—H9	120.2
C8—C7—C6	122.8 (4)	C8—C9—H9	120.2
C5—C4—C3	119.7 (4)	C7—C8—C9	119.2 (5)
C5—C4—H4	120.1	C7—C8—H8	120.4
C3—C4—H4	120.1	C9—C8—H8	120.4
N1—C1—C2	120.0 (5)	N2—C11—C10	124.1 (5)
N1—C1—H1	120.0	N2—C11—H11	118.0
C2—C1—H1	120.0	C10—C11—H11	118.0
C13—C18—C17	118.2 (5)	C9—C10—C11	117.9 (5)
C13—C18—H18	120.9	C9—C10—H10	121.1
C17—C18—H18	120.9	C11—C10—H10	121.1
C16—C15—C14	120.3 (5)	H1W1—O1—H1W2	92 (6)
Au1—S1—C12—N5	-157.3 (4)	N5—C13—C18—C17	-175.9 (4)
Au1—S1—C12—N4	23.6 (4)	C14—C15—C16—C17	0.4 (8)
N4—C12—N5—C13	176.7 (4)	C16—C15—C14—C13	0.7 (8)
S1—C12—N5—C13	-2.5 (7)	C18—C13—C14—C15	-0.6 (7)
N5—C12—N4—N3	-12.1 (6)	N5—C13—C14—C15	175.0 (4)
S1—C12—N4—N3	167.0 (3)	C15—C16—C17—C18	-1.6 (8)
C6—N3—N4—C12	177.8 (4)	C13—C18—C17—C16	1.6 (8)
C12—N5—C13—C18	-60.4 (7)	C5—C4—C3—C2	-0.1 (8)
C12—N5—C13—C14	124.1 (5)	N1—C1—C2—C3	1.7 (8)
N4—N3—C6—C7	-7.3 (6)	C4—C3—C2—C1	-1.5 (8)
N4—N3—C6—C5	173.0 (3)	C8—C7—N2—C11	-1.7 (6)
N1—C5—C6—N3	31.7 (5)	C6—C7—N2—C11	-179.8 (4)
C4—C5—C6—N3	-143.8 (4)	C2—C1—N1—C5	-0.2 (7)
N1—C5—C6—C7	-148.1 (4)	C4—C5—N1—C1	-1.4 (7)
C4—C5—C6—C7	36.4 (6)	C6—C5—N1—C1	-177.2 (4)
N3—C6—C7—N2	18.1 (6)	N2—C7—C8—C9	2.8 (7)
C5—C6—C7—N2	-162.1 (4)	C6—C7—C8—C9	-179.2 (4)
N3—C6—C7—C8	-160.0 (4)	C10—C9—C8—C7	-0.7 (7)
C5—C6—C7—C8	19.7 (6)	C7—N2—C11—C10	-1.6 (7)
N1—C5—C4—C3	1.5 (7)	C8—C9—C10—C11	-2.3 (8)
C6—C5—C4—C3	176.9 (4)	N2—C11—C10—C9	3.6 (8)
C14—C13—C18—C17	-0.5 (7)		

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N5—H5 <i>A</i> ...C12	0.86	2.46	3.246 (4)	153
N4—H4 <i>A</i> ...N2	0.86	1.97	2.629 (5)	133
N1—H1 <i>A</i> ...C12	0.80 (4)	2.26 (4)	2.989 (4)	150 (4)
O1—H1 <i>W</i> 1...C11 <sup>i</sup>	0.80 (2)	2.70 (5)	3.353 (4)	140 (6)
O1—H1 <i>W</i> 2...C12 <sup>ii</sup>	0.81 (2)	2.39 (2)	3.206 (4)	177 (6)
O2—H2 <i>W</i> 2...O1	0.82 (2)	2.06 (3)	2.855 (5)	163 (7)

Symmetry codes: (i)  $-x+1/2, -y+3/2, -z$ ; (ii)  $x, -y+1, z-1/2$ .