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(4-Chlorobenzoato)bis(5-methyl-2-pyridylamine)silver(I)

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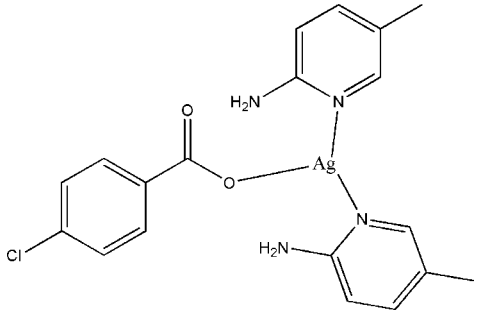
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.087; data-to-parameter ratio = 15.8.

The title compound, $[Ag(C_7H_4ClO_2)(C_6H_8N_2)_2]$, is a mononuclear silver(I) complex. The Ag^I atom is three-coordinated by two pyridine N atoms from two 5-methylpyridin-2-ylamine ligands and by one O atom of a 4-chlorobenzoate ligand, forming a distorted T-shaped coordination. In the crystal structure, the molecules are linked through intermolecular N—H···O hydrogen bonds, forming chains running along the b axis.

Related literature

For related literature, see: Bi *et al.* (2002); Deng *et al.* (2004); Jones *et al.* (2006); Khan *et al.* (2005); Kristiansson (2000); Li *et al.* (2007); Odoko *et al.* (2007); Sailaja *et al.* (2001); Wang & Okabe (2004).



Experimental

Crystal data

$[Ag(C_7H_4ClO_2)(C_6H_8N_2)_2]$
M_r = 479.71
Monoclinic, $P2_1/n$
a = 15.983 (3) Å
b = 5.7428 (9) Å
c = 21.703 (4) Å
β = 98.460 (2)°
V = 1970.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 298 (2) K
0.37 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.669, T_{max} = 0.704
13465 measured reflections
4064 independent reflections
3277 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 1.03
4064 reflections
258 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.179 (2)	Ag1—O1	2.647 (2)
Ag1—N3	2.193 (2)		
N1—Ag1—N3	151.99 (9)	N3—Ag1—O1	104.89 (9)
N1—Ag1—O1	103.05 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.88 (3)	2.11 (3)	2.977 (4)	169 (4)
N2—H2B···O2^{i}	0.89 (1)	1.94 (1)	2.822 (4)	174 (3)
N4—H4A···O1	0.88 (3)	2.09 (3)	2.966 (4)	167 (4)
N4—H4B···O1^{ii}	0.88 (1)	2.09 (3)	2.955 (3)	167 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2572).

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supporting information

Acta Cryst. (2008). E**64**, m591 [doi:10.1107/S1600536808008064]

(4-Chlorobenzoato)bis(5-methyl-2-pyridylamine)silver(I)

Yong-Qiang Tian, Tong Shen and Wu-Xia Liu

S1. Comment

Silver(I) complexes with carboxylate ligands and amine compounds have been widely investigated due to their versatile structures (Odoko *et al.*, 2007; Li *et al.*, 2007; Jones *et al.*, 2006; Bi *et al.*, 2002). We report herein the crystal structure of the title silver(I) complex.

The title compound is a mononuclear silver(I) complex (Fig. 1). The Ag^{I} atom is three-coordinated by two pyridine N atoms from two 5-methylpyridin-2-ylamine ligands and by one O atom of a 4-chlorobenzoate ligand, forming a distorted T-shaped coordination, the distortion being caused by the weak coordination of the carboxylate O atom (Ag1—O1 = 2.647 (2) Å, Table 1). The Ag—N bond lengths (Table 1) are comparable with the values observed in other silver(I) complexes (Kristiansson, 2000; Wang & Okabe, 2004; Sailaja *et al.*, 2001; Khan *et al.*, 2005; Deng *et al.*, 2004).

In the crystal structure, the molecules are linked through intermolecular N—H···O hydrogen bonds (Table 2), forming chains running along the *b* axis (Fig. 2).

S2. Experimental

Ag_2O (0.1 mmol, 23.2 mg) and 4-chlorobenzoic acid (0.1 mmol, 15.6 mg) were dissolved in an ammonia solution (10 ml, 30%), and the mixture was stirred for 20 min at room temperature. To the above mixture was added with stirring a methanol solution (3 ml) of 5-methylpyridin-2-ylamine (0.2 mmol, 21.6 mg). The final mixture was stirred for 30 min at room temperature. The resulting clear colourless solution was kept in dark for 12 d, yielding colourless block-shaped crystals.

S3. Refinement

Atoms H2A, H2B, H4A and H4B were located in a difference Fourier map and refined isotropically, with N—H and H···H distances restrained to 0.90 (1) Å and 1.43 (2) Å, respectively. Other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

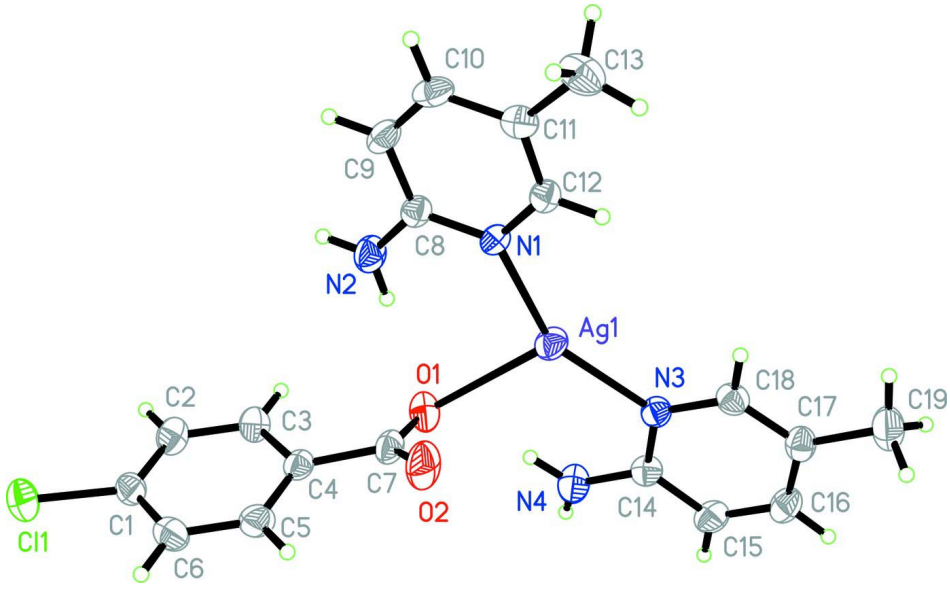

Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atomic numbering.

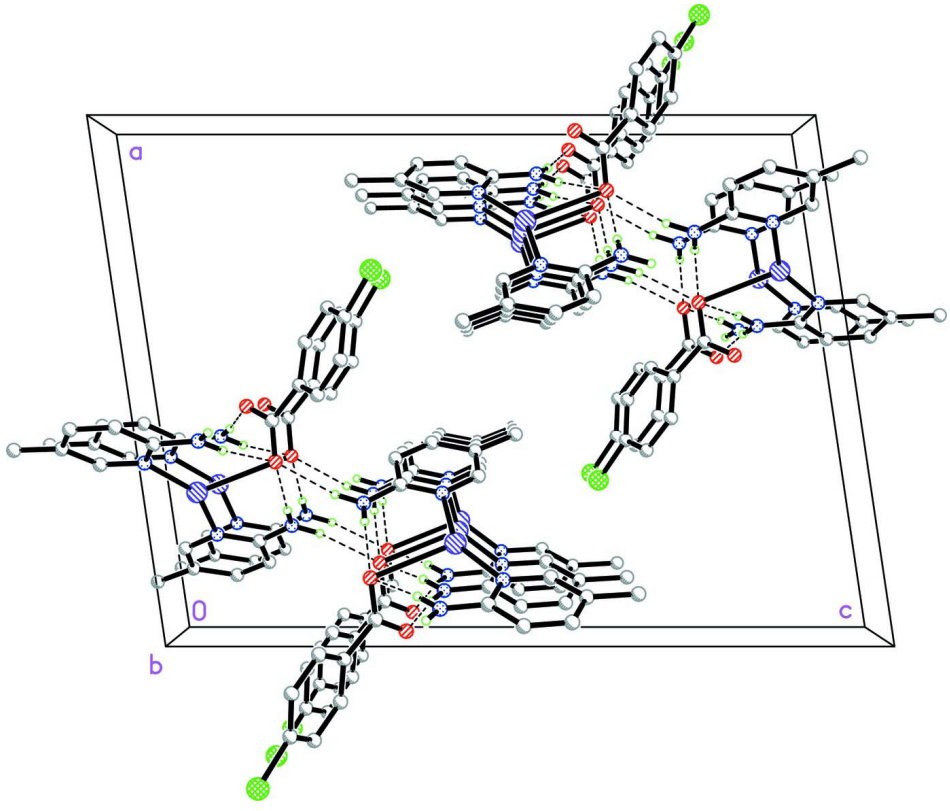

Figure 2

The crystal packing of the title compound, viewed down the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines.

(4-Chlorobenzoato)bis(5-methyl-2-pyridylamine)silver(I)

Crystal data

$[Ag(C_7H_4ClO_2)(C_6H_8N_2)_2]$
$M_r = 479.71$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.983$ (3) Å
$b = 5.7428$ (9) Å
$c = 21.703$ (4) Å
$\beta = 98.460$ (2)°
$V = 1970.4$ (6) Å^3
$Z = 4$
$F(000) = 968$
$D_x = 1.617$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3734 reflections
$\theta = 2.5$–24.9°
$\mu = 1.18$ mm^{-1}
$T = 298$ K
Block, colourless
0.37 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.669$, $T_{max} = 0.704$
13465 measured reflections
4064 independent reflections
3277 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.5°$
$h = -19 \rightarrow 20$
$k = -7 \rightarrow 7$
$l = -26 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.087$
$S = 1.03$
4064 reflections
258 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.4221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-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.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.291478 (15)	0.09298 (4)	0.077611 (11)	0.05012 (11)
Cl1	0.69700 (7)	0.65902 (19)	0.36548 (5)	0.0793 (3)
O1	0.35007 (14)	0.2179 (4)	0.19330 (10)	0.0573 (6)

O2	0.45197 (17)	0.0110 (5)	0.16007 (13)	0.0760 (8)
N1	0.34955 (14)	0.3452 (4)	0.02193 (11)	0.0388 (5)
N2	0.39194 (19)	0.5847 (5)	0.10583 (14)	0.0556 (7)
N3	0.20646 (14)	−0.2005 (4)	0.08709 (11)	0.0432 (6)
N4	0.2241 (2)	−0.1612 (6)	0.19393 (13)	0.0605 (8)
C1	0.6161 (2)	0.5050 (6)	0.31981 (14)	0.0507 (8)
C2	0.5373 (2)	0.6012 (6)	0.30750 (15)	0.0542 (8)
H2	0.5258	0.7432	0.3251	0.065*
C3	0.4749 (2)	0.4848 (6)	0.26869 (14)	0.0491 (7)
H3	0.4210	0.5489	0.2602	0.059*
C4	0.49170 (19)	0.2737 (5)	0.24224 (13)	0.0427 (7)
C5	0.5713 (2)	0.1802 (6)	0.25682 (16)	0.0554 (8)
H5	0.5831	0.0371	0.2400	0.066*
C6	0.6338 (2)	0.2935 (7)	0.29568 (17)	0.0631 (9)
H6	0.6873	0.2277	0.3054	0.076*
C7	0.4262 (2)	0.1546 (6)	0.19559 (14)	0.0481 (8)
C8	0.38570 (17)	0.5444 (5)	0.04449 (15)	0.0417 (7)
C9	0.41727 (18)	0.7050 (5)	0.00414 (17)	0.0501 (8)
H9	0.4412	0.8445	0.0198	0.060*
C10	0.41269 (19)	0.6557 (6)	−0.05702 (17)	0.0525 (8)
H10	0.4337	0.7613	−0.0834	0.063*
C11	0.37643 (19)	0.4460 (6)	−0.08121 (15)	0.0465 (7)
C12	0.34602 (17)	0.3021 (5)	−0.03981 (13)	0.0414 (7)
H12	0.3209	0.1636	−0.0551	0.050*
C13	0.3731 (2)	0.3791 (7)	−0.14840 (16)	0.0674 (11)
H13A	0.3471	0.2288	−0.1553	0.101*
H13B	0.4295	0.3734	−0.1586	0.101*
H13C	0.3406	0.4923	−0.1743	0.101*
C14	0.19164 (17)	−0.2802 (6)	0.14244 (14)	0.0438 (7)
C15	0.1459 (2)	−0.4866 (6)	0.14600 (16)	0.0535 (8)
H15	0.1354	−0.5405	0.1845	0.064*
C16	0.1171 (2)	−0.6072 (6)	0.09412 (17)	0.0548 (8)
H16	0.0872	−0.7447	0.0970	0.066*
C17	0.13206 (19)	−0.5268 (6)	0.03557 (15)	0.0493 (8)
C18	0.17643 (19)	−0.3242 (6)	0.03562 (15)	0.0477 (7)
H18	0.1868	−0.2669	−0.0026	0.057*
C19	0.1021 (3)	−0.6605 (7)	−0.02362 (18)	0.0726 (11)
H19A	0.1096	−0.5667	−0.0590	0.109*
H19B	0.0433	−0.6984	−0.0253	0.109*
H19C	0.1344	−0.8013	−0.0241	0.109*
H4B	0.209 (2)	−0.185 (6)	0.2308 (9)	0.080*
H4A	0.255 (2)	−0.032 (4)	0.1940 (16)	0.080*
H2B	0.407 (2)	0.720 (3)	0.1241 (14)	0.080*
H2A	0.374 (2)	0.489 (5)	0.1330 (13)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05372 (17)	0.04898 (17)	0.04972 (16)	−0.01056 (11)	0.01445 (11)	0.00527 (11)
Cl1	0.0798 (7)	0.0821 (7)	0.0669 (6)	−0.0191 (5)	−0.0192 (5)	−0.0079 (5)
O1	0.0522 (13)	0.0746 (17)	0.0462 (13)	−0.0174 (12)	0.0110 (10)	−0.0097 (12)
O2	0.0837 (18)	0.0637 (16)	0.0788 (18)	−0.0047 (14)	0.0062 (14)	−0.0372 (15)
N1	0.0404 (13)	0.0345 (13)	0.0426 (14)	−0.0033 (10)	0.0100 (10)	0.0007 (11)
N2	0.0648 (18)	0.0463 (17)	0.0552 (18)	−0.0051 (14)	0.0075 (14)	−0.0123 (14)
N3	0.0432 (13)	0.0454 (15)	0.0419 (14)	−0.0063 (11)	0.0090 (11)	0.0021 (12)
N4	0.0729 (19)	0.070 (2)	0.0420 (16)	−0.0249 (16)	0.0199 (14)	−0.0044 (15)
C1	0.060 (2)	0.054 (2)	0.0359 (16)	−0.0103 (17)	−0.0015 (14)	0.0007 (15)
C2	0.066 (2)	0.052 (2)	0.0465 (18)	−0.0065 (17)	0.0145 (16)	−0.0162 (15)
C3	0.0491 (18)	0.0522 (19)	0.0472 (18)	−0.0026 (15)	0.0113 (14)	−0.0094 (15)
C4	0.0540 (17)	0.0401 (17)	0.0349 (15)	−0.0079 (14)	0.0098 (13)	0.0005 (13)
C5	0.070 (2)	0.0414 (18)	0.053 (2)	0.0066 (17)	0.0023 (16)	−0.0042 (16)
C6	0.062 (2)	0.057 (2)	0.065 (2)	0.0071 (18)	−0.0105 (17)	0.0010 (19)
C7	0.063 (2)	0.0435 (18)	0.0385 (17)	−0.0144 (15)	0.0093 (15)	−0.0058 (14)
C8	0.0382 (15)	0.0341 (17)	0.0530 (18)	0.0034 (12)	0.0073 (13)	−0.0022 (14)
C9	0.0438 (17)	0.0309 (17)	0.076 (2)	0.0001 (13)	0.0093 (15)	0.0040 (16)
C10	0.0420 (17)	0.049 (2)	0.069 (2)	0.0037 (14)	0.0166 (15)	0.0233 (17)
C11	0.0390 (16)	0.054 (2)	0.0481 (18)	0.0057 (14)	0.0115 (13)	0.0076 (15)
C12	0.0390 (15)	0.0392 (17)	0.0466 (17)	−0.0012 (13)	0.0079 (12)	−0.0022 (14)
C13	0.061 (2)	0.097 (3)	0.046 (2)	0.001 (2)	0.0159 (17)	0.0094 (19)
C14	0.0403 (15)	0.0489 (19)	0.0448 (17)	−0.0016 (14)	0.0147 (13)	0.0035 (15)
C15	0.058 (2)	0.0520 (19)	0.054 (2)	−0.0088 (16)	0.0204 (15)	0.0091 (17)
C16	0.0476 (18)	0.047 (2)	0.072 (2)	−0.0092 (15)	0.0146 (16)	−0.0004 (17)
C17	0.0412 (16)	0.0497 (19)	0.057 (2)	−0.0005 (14)	0.0065 (14)	−0.0085 (16)
C18	0.0474 (17)	0.055 (2)	0.0409 (17)	−0.0020 (15)	0.0085 (13)	0.0045 (15)
C19	0.072 (2)	0.071 (3)	0.071 (3)	−0.008 (2)	−0.001 (2)	−0.021 (2)

Geometric parameters (Å, º)

Ag1—N1	2.179 (2)	C5—H5	0.93
Ag1—N3	2.193 (2)	C6—H6	0.93
Ag1—O1	2.647 (2)	C8—C9	1.415 (4)
Cl1—C1	1.748 (3)	C9—C10	1.348 (5)
O1—C7	1.263 (4)	C9—H9	0.93
O2—C7	1.240 (4)	C10—C11	1.404 (5)
N1—C8	1.342 (4)	C10—H10	0.93
N1—C12	1.356 (4)	C11—C12	1.362 (4)
N2—C8	1.340 (4)	C11—C13	1.501 (5)
N2—H2B	0.888 (10)	C12—H12	0.93
N2—H2A	0.88 (3)	C13—H13A	0.96
N3—C14	1.339 (4)	C13—H13B	0.96
N3—C18	1.351 (4)	C13—H13C	0.96
N4—C14	1.347 (4)	C14—C15	1.401 (4)
N4—H4B	0.883 (10)	C15—C16	1.344 (5)

N4—H4A	0.88 (3)	C15—H15	0.93
C1—C2	1.366 (5)	C16—C17	1.405 (5)
C1—C6	1.369 (5)	C16—H16	0.93
C2—C3	1.379 (4)	C17—C18	1.363 (5)
C2—H2	0.93	C17—C19	1.513 (5)
C3—C4	1.384 (4)	C18—H18	0.93
C3—H3	0.93	C19—H19A	0.96
C4—C5	1.375 (4)	C19—H19B	0.96
C4—C7	1.510 (4)	C19—H19C	0.96
C5—C6	1.373 (5)		

N1—Ag1—N3	151.99 (9)	C10—C9—C8	120.0 (3)
N1—Ag1—O1	103.05 (9)	C10—C9—H9	120.0
N3—Ag1—O1	104.89 (9)	C8—C9—H9	120.0
C8—N1—C12	118.0 (3)	C9—C10—C11	120.5 (3)
C8—N1—Ag1	124.1 (2)	C9—C10—H10	119.7
C12—N1—Ag1	117.89 (19)	C11—C10—H10	119.7
C8—N2—H2B	125 (2)	C12—C11—C10	116.2 (3)
C8—N2—H2A	125 (2)	C12—C11—C13	121.3 (3)
H2B—N2—H2A	110 (2)	C10—C11—C13	122.4 (3)
C14—N3—C18	118.3 (3)	N1—C12—C11	125.1 (3)
C14—N3—Ag1	122.7 (2)	N1—C12—H12	117.5
C18—N3—Ag1	118.44 (19)	C11—C12—H12	117.5
C14—N4—H4B	123 (2)	C11—C13—H13A	109.5
C14—N4—H4A	125 (2)	C11—C13—H13B	109.5
H4B—N4—H4A	111 (2)	H13A—C13—H13B	109.5
C2—C1—C6	121.4 (3)	C11—C13—H13C	109.5
C2—C1—Cl1	119.4 (3)	H13A—C13—H13C	109.5
C6—C1—Cl1	119.2 (3)	H13B—C13—H13C	109.5
C1—C2—C3	119.1 (3)	N3—C14—N4	118.2 (3)
C1—C2—H2	120.4	N3—C14—C15	120.1 (3)
C3—C2—H2	120.4	N4—C14—C15	121.6 (3)
C2—C3—C4	120.7 (3)	C16—C15—C14	120.5 (3)
C2—C3—H3	119.6	C16—C15—H15	119.8
C4—C3—H3	119.6	C14—C15—H15	119.8
C5—C4—C3	118.4 (3)	C15—C16—C17	120.4 (3)
C5—C4—C7	120.3 (3)	C15—C16—H16	119.8
C3—C4—C7	121.2 (3)	C17—C16—H16	119.8
C6—C5—C4	121.4 (3)	C18—C17—C16	115.9 (3)
C6—C5—H5	119.3	C18—C17—C19	122.3 (3)
C4—C5—H5	119.3	C16—C17—C19	121.8 (3)
C1—C6—C5	118.9 (3)	N3—C18—C17	124.8 (3)
C1—C6—H6	120.6	N3—C18—H18	117.6
C5—C6—H6	120.6	C17—C18—H18	117.6
O2—C7—O1	125.0 (3)	C17—C19—H19A	109.5
O2—C7—C4	117.2 (3)	C17—C19—H19B	109.5
O1—C7—C4	117.7 (3)	H19A—C19—H19B	109.5
N2—C8—N1	118.3 (3)	C17—C19—H19C	109.5

N2—C8—C9	121.4 (3)	H19A—C19—H19C	109.5
N1—C8—C9	120.2 (3)	H19B—C19—H19C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1	0.88 (3)	2.11 (3)	2.977 (4)	169 (4)
N2—H2*B*···O2^{i}	0.89 (1)	1.94 (1)	2.822 (4)	174 (3)
N4—H4*A*···O1	0.88 (3)	2.09 (3)	2.966 (4)	167 (4)
N4—H4*B*···O1^{ii}	0.88 (1)	2.09 (3)	2.955 (3)	167 (3)

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