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A one-dimensional silver(I) coordination polymer based on the 2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol ligand exhibiting photoluminescence

Dong-Cheng Hu, Chao-Hu Xiao, Guo-Zhe Guo, Yun-Xia Yang and Jia-Cheng Liu*

Key Laboratory of Polymer Materials of Gansu Province, Key Laboratory of Bioelectrochemtry and Environmental Analysis of Gansu College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070, People's Republic of China
Correspondence e-mail: jcliu8@163.com

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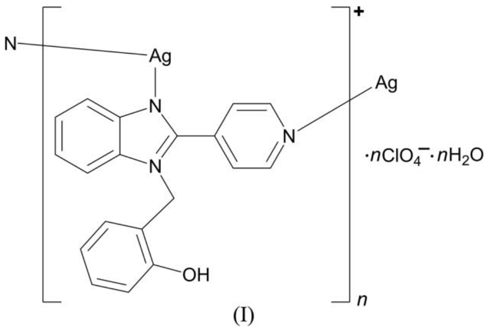
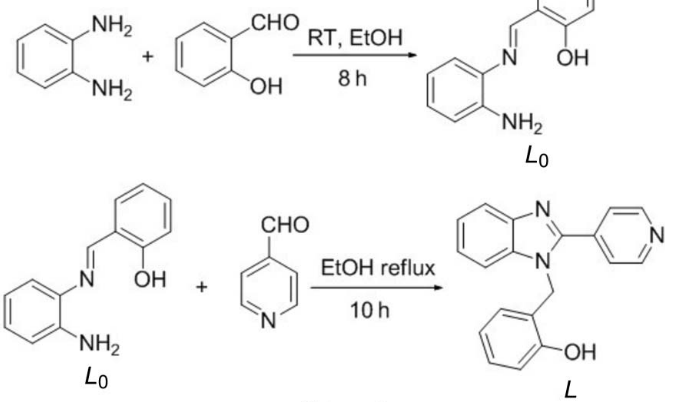
A one-dimensional Ag^I coordination complex, *catena*-poly-[[silver(I)-μ-{2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]-phenol-κ^2N^2:N^3}] perchlorate monohydrate], $\{[Ag(C_{19}H_{15}N_3O)]ClO_4\cdot H_2O\}_n$, was synthesized by the reaction of 2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol (L) with silver perchlorate. In the complex, the L ligands are arranged alternately and link Ag^I cations through one benzimidazole N atom and the N atom of the pyridine ring, leading to an extended zigzag chain structure. In addition, the one-dimensional chains are extended into a three-dimensional supramolecular architecture *via* O—H$\cdots$O hydrogen-bond interactions and π–π stacking interactions. The complex exhibits photoluminescence in acetonitrile solution, with an emission maximum at 390 nm, and investigation of the thermal stability reveals that the network structure is stable up to 650 K.

Comment

There is much interest in benzimidazole derivatives, due not only to their useful biological activities but also to their strong coordinating abilities as multidentate ligands (Kühler *et al.*, 2002; Carcanague *et al.*, 2002; Li *et al.*, 2007). It is well known that one common type of benzimidazole derivative comes from the transformation of symmetric Schiff base derivatives (Yang *et al.*, 2006). Such Schiff bases may conveniently be prepared by a one-step reaction of *o*-phenylenediamine with an aromatic aldehyde, but in refluxing ethanol they are usually converted into the benzimidazole derivatives. However, little attention has been paid to the transformation of unsymmetric Schiff base derivatives, since many factors influence the transformation process, including the ratio of *o*-phenylenediamine to aromatic aldehyde, and the reaction temperature. In our studies, we have synthesized the substituted benzimidazole ligand 2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol (L) derived from the transformation of an unsymmetric Schiff base (see Scheme 1). Within the ligand, the pyridine group is rigidly linked to the central C atom of the benzimidazole group, and the phenol group is attached *via* a –CH$_2$– group to an N atom (Kitazume & Ishikawa, 1974). The



(I)



Scheme 1

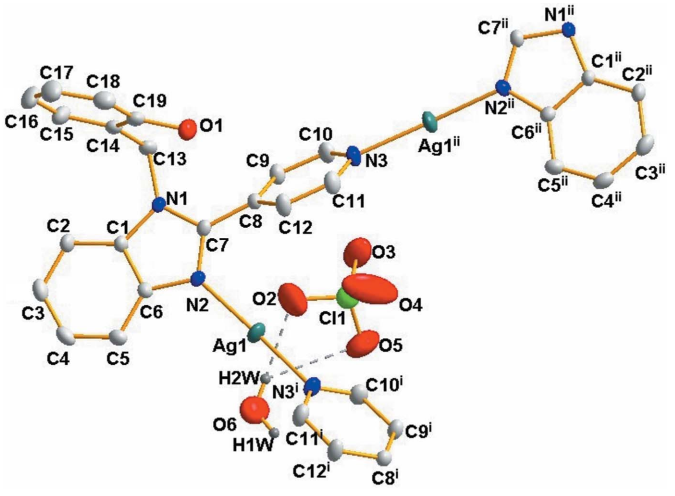


Figure 1
The Ag coordination environment of complex (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. [Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.]

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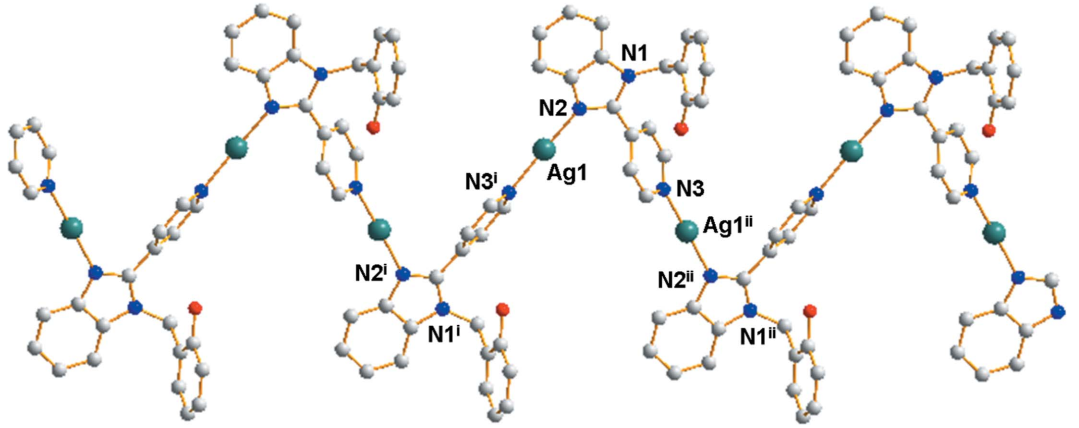

Figure 2
The one-dimensional coordination chain of (I). H atoms, water molecules and perchlorate anions have been omitted for clarity. The symmetry codes are as in Fig. 1.

title silver(I) complex, *catena*-poly[[silver(I)-μ-{2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol-κ^2N^2:N^3}] perchlorate monohydrate], (I), was obtained by the reaction of *L* with silver perchlorate.

Single-crystal X-ray diffraction reveals that complex (I) crystallizes in the monoclinic space group $P2_1/n$, with one Ag^{I} cation, one *L* ligand, a perchlorate anion and one solvent water molecule in the asymmetric unit. In (I), each Ag^{I} cation is coordinated by one N atom from each of two *L* ligands in a linear fashion (Fig. 1). Neighbouring Ag^{I} cations are bound together by pyridine atom N3 and benzimidazole atom N2 of the *L* ligand to form an $\{\mathrm{Ag}L\}_n$ one-dimensional zigzag chain (Fig. 2).

As the benzimidazole group is more electron-rich than pyridine, the Ag—N distance for the former [2.102 (3) Å] is slightly shorter than that for the latter [2.124 (3) Å], and the conformation of the *L* ligand is similar to that observed for related Ag^{I} complexes with benzimidazole and pyridine *N*-donor ligands (Xia *et al.*, 2005, 2007; Su *et al.*, 1999). The benzimidazole rings are almost coplanar in the zigzag chain, while the plane of the pyridine ring deviates from that of the benzimidazole ring with a dihedral angle of 53.97 (17)°. Atoms N2, Ag1 and N3^{i} [symmetry code: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$] are almost linear, with an N2—Ag1—N3^{i} angle of 173.76 (12)°, and the adjacent intra-chain atoms Ag1 and Ag1^{ii} [symmetry code: (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$] are bridged by the ligands with a separation of 6.936 (2) Å.

In the crystal packing of complex (I), two separate zigzag chains are connected by π–π interactions into a double chain, and the separation between neighbouring planes is 3.424 (2) Å (Fig. 3). In addition, the double-chain structures are extended into a three-dimensional supramolecular architecture along the *a* axis through interchain O—H$\cdots$O hydrogen-bonding interactions (Fig. 4) arising from the solvent water molecule (O6—H2*W*$\cdots$O2, O6—H2*W*$\cdots$O5, O6—H1*W*$\cdots$O3^{i} and O6—H1*W*$\cdots$O4^{i}; Table 1) and the hydroxy group of the *L* ligand (O1—H1$\cdots$O6^{iii}; Table 1).

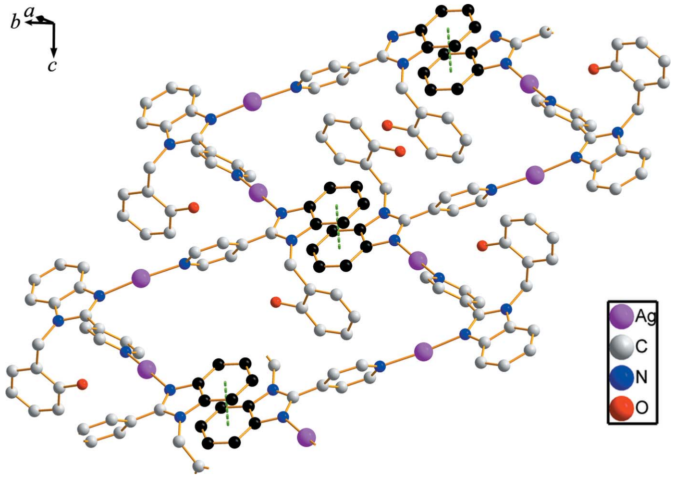

Figure 3
The π–π interactions (dashed lines) in (I).

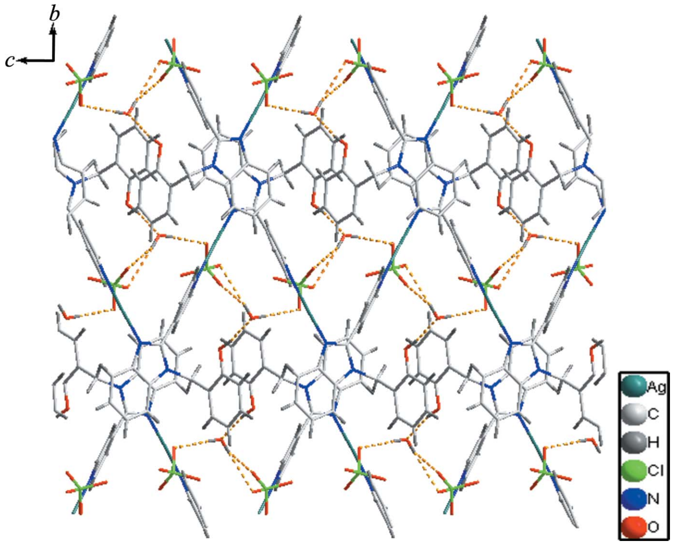

Figure 4
The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

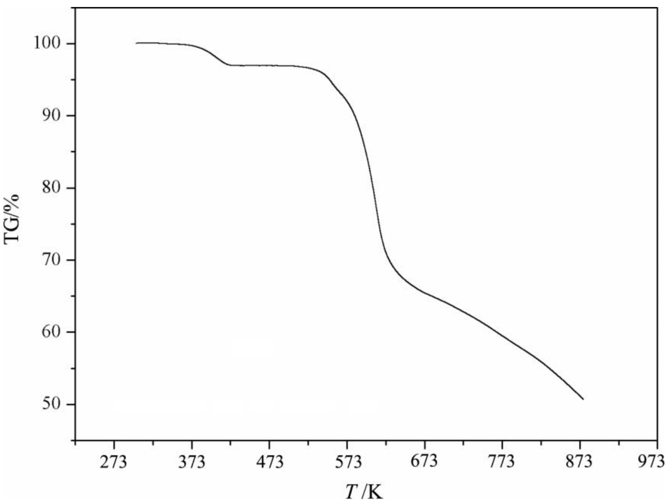

Figure 5
The thermogravimetric analysis (TGA) curve for (I).

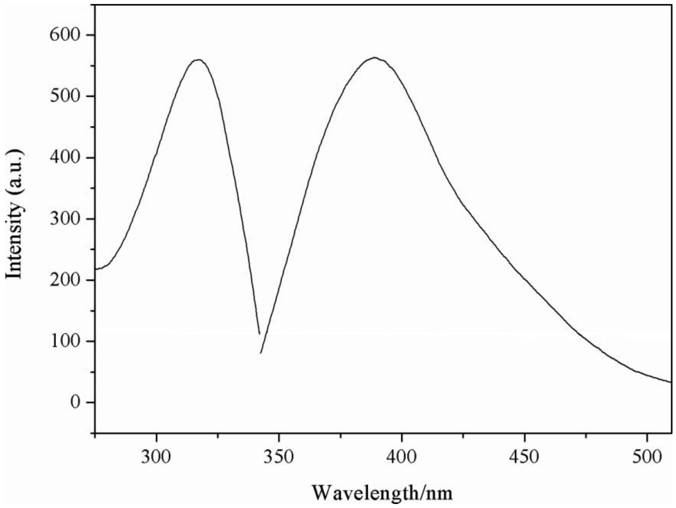

Figure 6
The photoluminescent spectrum of (I).

Thermogravimetric analysis (TGA) of the title polymer under an N_2 atmosphere with a heating rate of 10 K min^{-1} was investigated in the temperature range 303–873 K (Fig. 5). The TGA curve displays a weight loss of 3.2% at 353–423 K, which corresponds to the loss of the solvent water molecule. On heating above 506 K, a second weight loss of 19.5% is observed in the temperature range 506–650 K, which corresponds to the loss of the perchlorate anion. The framework starts to decompose at 650 K.

The free *L* ligand shows very weak luminescence (almost undetectable) in acetonitrile solution at ambient temperature. However, (I) does exhibit photoluminescence in acetonitrile solution at room temperature. Excitation of (I) at 320 nm produces a luminescence peak with a maximum at 390 nm (Fig. 6). This increase in the intensity of the luminescence may be attributed to the coordination of the *L* ligand to the Ag^I cation, which increases the rigidity of the *L* ligand and reduces the nonradiative relaxation process (Fang & Zhang, 2006).

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O6—H1$W\cdots$O3^{i}	0.84 (1)	2.57 (6)	3.217 (7)	135 (7)
O6—H1$W\cdots$O4^{i}	0.84 (1)	2.48 (2)	3.316 (9)	169 (9)
O1—H1$\cdots$O6^{ii}	0.82	1.91	2.721 (5)	170
O6—H2$W\cdots$O2	0.84 (1)	2.23 (5)	2.973 (8)	146 (9)
O6—H2$W\cdots$O5	0.84 (1)	2.57 (4)	3.363 (9)	157 (7)

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

Experimental

2-[2-(Pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol (*L*) was synthesized according to a modification of a previously reported procedure (Fellah *et al.*, 2010). To a solution of *o*-phenylenediamine (2.16 g, 20 mmol) in ethanol (20 ml), 2-hydroxybenzaldehyde (1.22 g, 10 mmol) dissolved in ethanol (10 ml) was added dropwise. The mixture was stirred at room temperature for 8 h. A yellow precipitate formed and was isolated by filtration. The crude product, L_0 (see Scheme 1), was then crystallized from ethanol. A solution of L_0 (2.12 g, 10 mmol) and pyridine-4-carbaldehyde (1.07 g, 10 mmol) in ethanol (50 ml) was heated for 10 h under reflux. The reaction mixture was cooled, and a white precipitate of *L* formed and was filtered off (yield 71 wt%).

To a solution of *L* (0.1 mmol, 30.1 mg) in a mixture (10 ml) of methanol and tetrahydrofuran (1:1 *v*/*v*), $AgClO_4$ (21 mg, 0.1 mmol) was added. After stirring at room temperature for 30 min, $NH_3{\cdot}H_2O$ (2 ml) was added dropwise. The mixture was stirred for another 30 min and then filtered. Colourless block-shaped crystals of (I) were obtained by evaporation after one week (yield 40 wt%, based on *L*). Analysis calculated for $C_{19}H_{17}AgClN_3O_6$: C 43.33, H 3.25, N 7.98%; found: C 43.81, H 3.11, N 7.64%. FT–IR (KBr, ν, cm^{-1}): 3454 (*s*), 3058 (*s*), 2951 (*s*), 2860 (*s*), 2727 (*s*), 2609 (*s*), 1604 (*m*), 1506 (*w*), 1444 (*s*), 1412 (*s*), 1273 (*m*), 1241 (*m*), 1156 (*w*), 1070 (*m*), 984 (*w*), 909 (*w*), 835 (*m*), 749 (*m*), 674 (*w*), 589 (*w*), 535 (*w*).

Crystal data

$[Ag(C_{19}H_{15}N_3O)]ClO_4{\cdot}H_2O$
M_r = 526.68
Monoclinic, $P2_1/n$
a = 9.739 (3) Å
b = 21.260 (7) Å
c = 9.952 (3) Å
β = 103.851 (3)°
V = 2000.8 (11) $Å^3$
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 296 K
0.23 × 0.21 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.772, T_{max} = 0.833
10711 measured reflections
3712 independent reflections
3023 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.12
3712 reflections
280 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.68 e $Å^{-3}$

The hydroxy H atom was positioned and refined by a freely rotating O—H bond and with a fixed distance of O—H = 0.82 Å and with $U_{iso}(H) = 1.5U_{eq}(O)$. The water H atoms were located from difference Fourier maps and refined isotropically with O—H and H···H distance restraints of 0.84 (1) and 1.48 (1) Å, respectively. The remaining H atoms were included in calculated positions and refined in the riding-model approximation, with C—H = 0.93 or 0.97 Å for methine and methylene H atoms, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: WQ3027). Services for accessing these data are described at the back of the journal.

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supplementary materials

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catena-Poly[[silver(I)-μ-{2-[2-(pyridin-4-yl)-1*H*-benzimidazol-1-ylmethyl]phenol-κ^2N^2:N^3}] perchlorate monohydrate]

Crystal data

$[Ag(C_{19}H_{15}N_3O)]ClO_4\cdot H_2O$
M_r = 526.68
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Hall symbol: -P 2yn
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β = 103.851 (3)°
V = 2000.8 (11) Å^3
Z = 4
$F(000)$ = 1056
D_x = 1.748 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5048 reflections
θ = 2.3–28.2°
μ = 1.18 mm^{-1}
T = 296 K
Block, colourless
0.23 × 0.21 × 0.16 mm

Data collection

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Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.772, T_{max} = 0.833
10711 measured reflections
3712 independent reflections
3023 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.5°, θ_{min} = 2.3°
$h = -11\rightarrow 9$
$k = -25\rightarrow 25$
$l = -11\rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.12
3712 reflections
280 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 2.8471P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 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 (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Ag1	0.11957 (4)	0.828815 (14)	0.37908 (4)	0.04760 (13)
C1	0.2473 (4)	1.01422 (15)	0.5315 (4)	0.0282 (7)
C2	0.2306 (4)	1.07915 (17)	0.5172 (4)	0.0349 (8)
H2	0.2886	1.1068	0.5777	0.042*
C3	0.1241 (4)	1.10039 (19)	0.4095 (4)	0.0439 (10)
H3	0.1095	1.1434	0.3969	0.053*
C4	0.0378 (4)	1.05856 (19)	0.3187 (4)	0.0423 (10)
H4	−0.0332	1.0746	0.2472	0.051*
C5	0.0544 (4)	0.99477 (18)	0.3315 (4)	0.0361 (9)
H5	−0.0032	0.9672	0.2702	0.043*
C6	0.1614 (4)	0.97299 (16)	0.4406 (4)	0.0286 (8)
C7	0.3071 (4)	0.91684 (15)	0.5924 (4)	0.0268 (7)
C8	0.3816 (4)	0.86186 (16)	0.6642 (4)	0.0286 (8)
C9	0.5260 (4)	0.85504 (17)	0.6840 (4)	0.0363 (9)
H9	0.5796	0.8868	0.6572	0.044*
C10	0.5902 (4)	0.80058 (18)	0.7443 (4)	0.0414 (9)
H10	0.6874	0.7961	0.7561	0.050*
C11	0.3788 (5)	0.76084 (18)	0.7658 (5)	0.0450 (10)
H11	0.3274	0.7285	0.7934	0.054*
C12	0.3076 (4)	0.81321 (17)	0.7063 (5)	0.0394 (9)
H12	0.2101	0.8160	0.6942	0.047*
C13	0.4355 (4)	1.00207 (17)	0.7557 (4)	0.0354 (8)
H13A	0.4961	1.0343	0.7318	0.042*
H13B	0.4954	0.9682	0.8019	0.042*
C14	0.3540 (4)	1.02929 (17)	0.8527 (4)	0.0338 (8)
C15	0.3435 (5)	1.09382 (19)	0.8697 (4)	0.0493 (11)
H15	0.3905	1.1209	0.8225	0.059*
C16	0.2652 (6)	1.1182 (2)	0.9550 (5)	0.0660 (15)
H16	0.2586	1.1615	0.9649	0.079*
C17	0.1972 (6)	1.0787 (2)	1.0249 (5)	0.0615 (13)
H17	0.1422	1.0954	1.0808	0.074*
C18	0.2084 (5)	1.0143 (2)	1.0143 (4)	0.0482 (10)
H18	0.1640	0.9877	1.0649	0.058*
C19	0.2866 (4)	0.98963 (18)	0.9273 (4)	0.0368 (9)
Cl1	0.48617 (13)	0.76977 (6)	0.34110 (14)	0.0599 (3)
N1	0.3401 (3)	0.97766 (13)	0.6279 (3)	0.0270 (6)
N2	0.2016 (3)	0.91201 (13)	0.4816 (3)	0.0285 (6)

N3	0.5181 (4)	0.75419 (14)	0.7861 (4)	0.0393 (8)
O1	0.3008 (3)	0.92688 (13)	0.9095 (3)	0.0482 (7)
H1	0.2722	0.9077	0.9689	0.072*
O2	0.4204 (6)	0.8299 (3)	0.3398 (6)	0.136 (2)
O3	0.6273 (4)	0.7772 (2)	0.4112 (5)	0.0911 (14)
O4	0.4202 (7)	0.7306 (4)	0.4127 (7)	0.204 (4)
O5	0.4690 (7)	0.7535 (3)	0.2017 (5)	0.129 (2)
O6	0.1963 (7)	0.8518 (2)	0.0830 (5)	0.0896 (13)
H1W	0.133 (6)	0.830 (3)	0.032 (8)	0.18 (5)*
H2W	0.272 (5)	0.836 (3)	0.131 (9)	0.17 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0518 (2)	0.03009 (17)	0.0568 (2)	−0.01082 (14)	0.00479 (15)	−0.01380 (14)
C1	0.0305 (19)	0.0242 (17)	0.0293 (18)	−0.0004 (15)	0.0059 (15)	0.0016 (14)
C2	0.040 (2)	0.0241 (17)	0.040 (2)	−0.0033 (16)	0.0093 (18)	0.0014 (15)
C3	0.051 (3)	0.032 (2)	0.052 (3)	0.0102 (18)	0.019 (2)	0.0128 (18)
C4	0.040 (2)	0.048 (2)	0.037 (2)	0.0094 (19)	0.0057 (18)	0.0140 (18)
C5	0.032 (2)	0.043 (2)	0.0312 (19)	0.0031 (17)	0.0038 (16)	−0.0002 (16)
C6	0.033 (2)	0.0268 (17)	0.0265 (18)	0.0000 (15)	0.0078 (15)	0.0023 (14)
C7	0.0264 (18)	0.0231 (16)	0.0324 (18)	−0.0013 (14)	0.0102 (15)	−0.0015 (14)
C8	0.0299 (19)	0.0253 (17)	0.0309 (18)	0.0034 (14)	0.0078 (15)	−0.0006 (14)
C9	0.035 (2)	0.0284 (18)	0.048 (2)	0.0023 (16)	0.0134 (18)	0.0056 (16)
C10	0.033 (2)	0.036 (2)	0.054 (3)	0.0060 (17)	0.0102 (19)	0.0031 (18)
C11	0.046 (3)	0.0297 (19)	0.063 (3)	0.0021 (18)	0.020 (2)	0.0111 (19)
C12	0.029 (2)	0.0287 (19)	0.063 (3)	0.0019 (16)	0.0163 (19)	0.0063 (18)
C13	0.032 (2)	0.0344 (19)	0.035 (2)	−0.0082 (16)	−0.0021 (16)	−0.0031 (16)
C14	0.034 (2)	0.0335 (19)	0.0284 (19)	−0.0004 (16)	−0.0025 (16)	−0.0037 (15)
C15	0.073 (3)	0.033 (2)	0.039 (2)	−0.006 (2)	0.008 (2)	−0.0057 (17)
C16	0.105 (4)	0.043 (3)	0.050 (3)	0.011 (3)	0.019 (3)	−0.014 (2)
C17	0.076 (4)	0.065 (3)	0.045 (3)	0.017 (3)	0.018 (2)	−0.011 (2)
C18	0.049 (3)	0.058 (3)	0.037 (2)	−0.001 (2)	0.010 (2)	0.0002 (19)
C19	0.036 (2)	0.038 (2)	0.030 (2)	−0.0013 (17)	−0.0040 (16)	−0.0030 (16)
Cl1	0.0478 (7)	0.0585 (7)	0.0742 (8)	−0.0142 (6)	0.0164 (6)	−0.0028 (6)
N1	0.0289 (16)	0.0227 (14)	0.0278 (15)	−0.0018 (12)	0.0035 (13)	−0.0018 (11)
N2	0.0279 (16)	0.0259 (14)	0.0309 (16)	−0.0001 (12)	0.0053 (13)	−0.0049 (12)
N3	0.0394 (19)	0.0304 (16)	0.047 (2)	0.0085 (14)	0.0088 (16)	0.0065 (14)
O1	0.063 (2)	0.0341 (15)	0.0473 (17)	−0.0035 (14)	0.0128 (15)	0.0020 (13)
O2	0.147 (5)	0.157 (5)	0.104 (4)	0.096 (4)	0.030 (3)	0.002 (3)
O3	0.044 (2)	0.093 (3)	0.137 (4)	−0.012 (2)	0.024 (2)	−0.028 (3)
O4	0.149 (5)	0.274 (8)	0.149 (5)	−0.160 (6)	−0.041 (4)	0.108 (6)
O5	0.177 (5)	0.118 (4)	0.088 (3)	−0.012 (4)	0.020 (3)	−0.045 (3)
O6	0.109 (4)	0.079 (3)	0.078 (3)	−0.021 (3)	0.018 (3)	0.021 (2)

Geometric parameters (Å, º)

Ag1—N2	2.102 (3)	C12—H12	0.9300
Ag1—N3^{i}	2.124 (3)	C13—N1	1.479 (4)
C1—C6	1.387 (5)	C13—C14	1.505 (5)

C1—N1	1.388 (4)	C13—H13A	0.9700
C1—C2	1.393 (5)	C13—H13B	0.9700
C2—C3	1.377 (5)	C14—C19	1.388 (5)
C2—H2	0.9300	C14—C15	1.389 (5)
C3—C4	1.396 (6)	C15—C16	1.372 (7)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.368 (6)	C16—C17	1.359 (7)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.392 (5)	C17—C18	1.379 (7)
C5—H5	0.9300	C17—H17	0.9300
C6—N2	1.387 (4)	C18—C19	1.386 (6)
C7—N2	1.319 (4)	C18—H18	0.9300
C7—N1	1.358 (4)	C19—O1	1.357 (5)
C7—C8	1.468 (5)	Cl1—O4	1.354 (5)
C8—C9	1.380 (5)	Cl1—O3	1.393 (4)
C8—C12	1.381 (5)	Cl1—O5	1.400 (5)
C9—C10	1.382 (5)	Cl1—O5	1.400 (5)
C9—H9	0.9300	Cl1—O2	1.428 (5)
C10—N3	1.334 (5)	Cl1—O2	1.428 (5)
C10—H10	0.9300	N3—Ag1^{ii}	2.124 (3)
C11—N3	1.331 (5)	O1—H1	0.8200
C11—C12	1.369 (5)	O6—H1W	0.842 (10)
C11—H11	0.9300	O6—H2W	0.843 (10)

N2—Ag1—N3^{i}	173.76 (12)	C19—C14—C15	118.5 (4)
C6—C1—N1	106.8 (3)	C19—C14—C13	120.0 (3)
C6—C1—C2	121.5 (3)	C15—C14—C13	121.6 (4)
N1—C1—C2	131.8 (3)	C16—C15—C14	121.1 (4)
C3—C2—C1	116.9 (4)	C16—C15—H15	119.4
C3—C2—H2	121.6	C14—C15—H15	119.4
C1—C2—H2	121.6	C17—C16—C15	119.6 (4)
C2—C3—C4	121.3 (4)	C17—C16—H16	120.2
C2—C3—H3	119.4	C15—C16—H16	120.2
C4—C3—H3	119.4	C16—C17—C18	121.1 (5)
C5—C4—C3	122.1 (4)	C16—C17—H17	119.4
C5—C4—H4	118.9	C18—C17—H17	119.4
C3—C4—H4	118.9	C17—C18—C19	119.3 (4)
C4—C5—C6	116.9 (4)	C17—C18—H18	120.4
C4—C5—H5	121.6	C19—C18—H18	120.4
C6—C5—H5	121.6	O1—C19—C18	122.8 (4)
N2—C6—C1	108.3 (3)	O1—C19—C14	116.8 (4)
N2—C6—C5	130.3 (3)	C18—C19—C14	120.4 (4)
C1—C6—C5	121.4 (3)	O4—Cl1—O3	110.0 (3)
N2—C7—N1	112.3 (3)	O4—Cl1—O5	114.2 (4)
N2—C7—C8	122.7 (3)	O3—Cl1—O5	113.2 (3)
N1—C7—C8	125.0 (3)	O4—Cl1—O5	114.2 (4)
C9—C8—C12	117.7 (3)	O3—Cl1—O5	113.2 (3)
C9—C8—C7	121.4 (3)	O4—Cl1—O2	106.7 (5)
C12—C8—C7	120.7 (3)	O3—Cl1—O2	106.9 (3)

C8—C9—C10	119.3 (4)	O5—Cl1—O2	105.3 (3)
C8—C9—H9	120.3	O5—Cl1—O2	105.3 (3)
C10—C9—H9	120.3	O4—Cl1—O2	106.7 (5)
N3—C10—C9	122.5 (4)	O3—Cl1—O2	106.9 (3)
N3—C10—H10	118.8	O5—Cl1—O2	105.3 (3)
C9—C10—H10	118.8	O5—Cl1—O2	105.3 (3)
N3—C11—C12	123.0 (4)	C7—N1—C1	106.2 (3)
N3—C11—H11	118.5	C7—N1—C13	128.2 (3)
C12—C11—H11	118.5	C1—N1—C13	124.7 (3)
C11—C12—C8	119.6 (4)	C7—N2—C6	106.4 (3)
C11—C12—H12	120.2	C7—N2—Ag1	126.9 (2)
C8—C12—H12	120.2	C6—N2—Ag1	126.6 (2)
N1—C13—C14	111.5 (3)	C11—N3—C10	117.9 (3)
N1—C13—H13A	109.3	C11—N3—Ag1^{ii}	120.4 (3)
C14—C13—H13A	109.3	C10—N3—Ag1^{ii}	121.7 (3)
N1—C13—H13B	109.3	C19—O1—H1	109.5
C14—C13—H13B	109.3	H1W—O6—H2W	122 (2)
H13A—C13—H13B	108.0		

C6—C1—C2—C3	0.5 (6)	C17—C18—C19—C14	0.6 (6)
N1—C1—C2—C3	−178.7 (4)	C15—C14—C19—O1	−179.1 (4)
C1—C2—C3—C4	−0.3 (6)	C13—C14—C19—O1	1.1 (5)
C2—C3—C4—C5	−0.2 (6)	C15—C14—C19—C18	1.4 (6)
C3—C4—C5—C6	0.4 (6)	C13—C14—C19—C18	−178.4 (4)
N1—C1—C6—N2	0.1 (4)	N2—C7—N1—C1	0.2 (4)
C2—C1—C6—N2	−179.3 (3)	C8—C7—N1—C1	178.2 (3)
N1—C1—C6—C5	179.1 (3)	N2—C7—N1—C13	169.8 (3)
C2—C1—C6—C5	−0.3 (6)	C8—C7—N1—C13	−12.2 (6)
C4—C5—C6—N2	178.5 (4)	C6—C1—N1—C7	−0.2 (4)
C4—C5—C6—C1	−0.2 (6)	C2—C1—N1—C7	179.1 (4)
N2—C7—C8—C9	123.2 (4)	C6—C1—N1—C13	−170.2 (3)
N1—C7—C8—C9	−54.6 (5)	C2—C1—N1—C13	9.1 (6)
N2—C7—C8—C12	−52.6 (5)	C14—C13—N1—C7	−104.0 (4)
N1—C7—C8—C12	129.6 (4)	C14—C13—N1—C1	63.8 (4)
C12—C8—C9—C10	0.1 (6)	N1—C7—N2—C6	−0.1 (4)
C7—C8—C9—C10	−175.9 (3)	C8—C7—N2—C6	−178.1 (3)
C8—C9—C10—N3	−0.9 (6)	N1—C7—N2—Ag1	176.1 (2)
N3—C11—C12—C8	0.2 (7)	C8—C7—N2—Ag1	−2.0 (5)
C9—C8—C12—C11	0.3 (6)	C5—C6—N2—C7	−178.9 (4)
C7—C8—C12—C11	176.2 (4)	C1—C6—N2—Ag1	−176.2 (2)
N1—C13—C14—C19	74.4 (4)	C5—C6—N2—Ag1	4.9 (6)
N1—C13—C14—C15	−105.4 (4)	N3^{i}—Ag1—N2—C7	103.2 (11)
C19—C14—C15—C16	−1.9 (6)	N3^{i}—Ag1—N2—C6	−81.3 (12)
C13—C14—C15—C16	177.9 (4)	C12—C11—N3—C10	−0.9 (6)
C14—C15—C16—C17	0.4 (8)	C12—C11—N3—Ag1^{ii}	−179.9 (3)
C15—C16—C17—C18	1.6 (8)	C9—C10—N3—C11	1.3 (6)
C16—C17—C18—C19	−2.1 (7)	C9—C10—N3—Ag1^{ii}	−179.7 (3)
C17—C18—C19—O1	−178.9 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H1*W*···O3^{i}	0.84 (1)	2.57 (6)	3.217 (7)	135 (7)
O6—H1*W*···O4^{i}	0.84 (1)	2.48 (2)	3.316 (9)	169 (9)
O1—H1···O6^{iii}	0.82	1.91	2.721 (5)	170
O6—H2*W*···O2	0.84 (1)	2.23 (5)	2.973 (8)	146 (9)
O6—H2*W*···O5	0.84 (1)	2.57 (4)	3.363 (9)	157 (7)

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