

Bis[μ -4'-[4-(quinolin-8-yloxymethyl)-phenyl]-2,2':6',2''-terpyridine}disilver(I) bis(perchlorate) dimethylformamide disolvate

Chang-Juan Chen, Feng-Neng Liu, Ai-Jiang Zhang, Liang-Wei Zhang and Xiang Liu*

State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, People's Republic of China

Correspondence e-mail: liuxiang@lzu.edu.cn

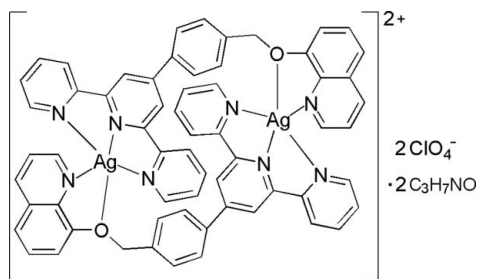
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 19.0.

In the binuclear title complex, $[\text{Ag}_2(\text{C}_{31}\text{H}_{22}\text{N}_4\text{O})_2](\text{ClO}_4)_2 \cdot 2\text{C}_3\text{H}_7\text{NO}$, the Ag^{I} atom is pentacoordinated by three N atoms from the tridentate chelating terpyridyl group and by one N atom and one O atom from the quinolin-8-yloxy group in a distorted square-pyramidal geometry with the O atom at the apical position. The centrosymmetric complex cation involves intramolecular $\pi-\pi$ stacking interactions [centroid-centroid distance = 3.862 (4) Å] between the central pyridine and benzene rings. In the crystal structure, intermolecular C—H \cdots O hydrogen bonds result in the formation of a supra-molecular network.

Related literature

For applications of 2,2':6',2''-terpyridine in supramolecular frameworks and functional materials, see: Andres & Schubert (2004); Constable *et al.* (2005); Thompson (1997); Ziener *et al.* (2000). For the ligand synthesis, see: Chow *et al.* (2006). For related structures, see: Hou & Li (2005).



Experimental

Crystal data

$[\text{Ag}_2(\text{C}_{31}\text{H}_{22}\text{N}_4\text{O})_2](\text{ClO}_4)_2 \cdot 2\text{C}_3\text{H}_7\text{NO}$
 $M_r = 1493.88$
 Monoclinic, $P2_1/c$
 $a = 10.0552$ (16) Å
 $b = 10.9548$ (18) Å
 $c = 29.657$ (5) Å
 $\beta = 96.767$ (8) $^\circ$
 $V = 3244.0$ (9) Å 3
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.76$ mm $^{-1}$
 $T = 296$ K
 $0.22 \times 0.20 \times 0.20$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.847$, $T_{\text{max}} = 0.860$
 20993 measured reflections
 8077 independent reflections
 5406 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.118$
 $S = 1.03$
 8077 reflections
 426 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.67$ e Å $^{-3}$
 $\Delta\rho_{\text{min}} = -0.44$ e Å $^{-3}$

Table 1

Selected bond lengths (Å).

Ag1—O1	2.5995 (19)	Ag1—N3	2.414 (3)
Ag1—N1	2.434 (3)	Ag1—N4	2.275 (2)
Ag1—N2	2.3572 (19)		

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 \cdots O3 $^{\text{i}}$	0.93	2.57	3.450 (5)	158
C12—H12 \cdots O5 $^{\text{ii}}$	0.93	2.60	3.344 (5)	138
C28—H28 \cdots O6 $^{\text{iii}}$	0.93	2.37	3.250 (5)	158
C29—H29 \cdots O4	0.93	2.57	3.252 (6)	130

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); 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: HY2238).

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supplementary materials

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Bis{ μ -4'-[4-(quinolin-8-yloxymethyl)phenyl]-2,2':6',2''-terpyridine}disilver(I) bis(perchlorate) dimethylformamide disolvate

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Comment

2,2':6',2''-Terpyridine is well known for its applications in the synthesis of supramolecular frameworks and functional materials (Andres & Schubert, 2004; Constable *et al.*, 2005; Thompson, 1997; Ziener *et al.*, 2000). Therefore, it is necessary to further widen the system of multifunctional terpyridyl derivatives complexes. Herein we report the synthesis and structure of an Ag^I complex with a new ligand 4'-[4'-(8-oxyquinoline)benzyl]-2,2':6',2''-terpyridine.

The complex cation of the title compound has a twisted box structure formed by two ligands bridging two Ag^I atoms. The asymmetric unit consists of a half of the cation, one perchlorate anion and one dimethylformamide solvent molecule. As shown Fig. 1, the two ligands are arranged in a head-to-tail fashion. The Ag^I atom is pentacoordinated by three N atoms of the tridentate chelating terpyridyl group and by one N and one O atoms from the quinolin-8-yloxy group [Ag—N = 2.275 (2)–2.434 (3) Å and Ag—O = 2.5995 (19) Å] (Table 1). The Ag⁺···Ag distance is 10.744 (6) Å in the dimeric complex cation. The plane of the 4'-phenyl-2,2':6',2''-terpyridine group is almost perpendicular to that of the quinoline group, with a dihedral angle of 79.96 (1)°. The complex cation involves π – π stacking interactions [centroid–centroid distance = 3.862 (4) Å] between the central pyridine rings and the phenyl rings. In the crystal structure, intermolecular C—H···O hydrogen bonds result in the formation of a supramolecular network (Table 2 and Fig. 2).

Experimental

The ligand was synthesized according to the literature (Chow *et al.*, 2006). A solution of AgClO₄ (23.72 mg, 0.10 mmol) in CH₃OH (10 ml) was added to a solution of the ligand (46.6 mg, 0.10 mmol) in CHCl₃ (10 ml) with stirring. The brown precipitate was collected by filtration and washed sequentially with 10 ml CH₃OH and CHCl₃. Brown crystals suitable for X-ray structure determination were obtained by slow diffusion of diethyl ether into the DMF solution of the product in several days.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (CH₂) and 0.96 (CH₃) Å and with $U_{\text{iso}} = 1.2(1.5 \text{ for methyl})U_{\text{eq}}(\text{C})$.

Figures

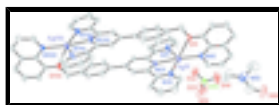


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (A) 2 - z, 1 - y, 1 - z.]

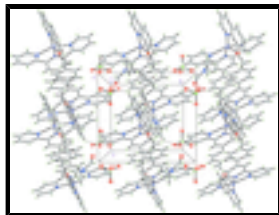


Fig. 2. Packing diagram along the *c* axis of the title compound. Hydrogen bonds are shown as dashed lines.

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Crystal data

[Ag₂(C₃₁H₂₂N₄O)₂](ClO₄)₂·2C₃H₇NO

M_r = 1493.88

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 10.0552 (16) Å

b = 10.9548 (18) Å

c = 29.657 (5) Å

β = 96.767 (8)°

V = 3244.0 (9) Å³

Z = 2

F(000) = 1520

D_x = 1.529 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 6845 reflections

θ = 2.3–28.6°

μ = 0.76 mm⁻¹

T = 296 K

Block, yellow

0.22 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

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

T_{min} = 0.847, *T_{max}* = 0.860

20993 measured reflections

8077 independent reflections

5406 reflections with *I* > 2σ(*I*)

R_{int} = 0.020

θ_{max} = 28.7°, θ_{min} = 2.0°

h = -12→12

k = -14→14

l = -40→28

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.041

wR(*F*²) = 0.118

S = 1.03

8077 reflections

426 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0551*P*)² + 1.1422*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.67 e Å⁻³

0 restraints

$$\Delta\rho_{\min} = -0.44 \text{ e } \text{\AA}^{-3}$$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.60078 (2)	0.42357 (2)	0.602143 (7)	0.06913 (11)
C1	0.6898 (5)	0.1295 (4)	0.61912 (13)	0.1029 (14)
H1	0.6456	0.1402	0.6447	0.123*
C2	0.7329 (5)	0.0155 (4)	0.60987 (14)	0.1074 (15)
H2	0.7210	-0.0493	0.6293	0.129*
C3	0.7939 (4)	-0.0024 (3)	0.57173 (14)	0.0904 (12)
H3	0.8235	-0.0795	0.5645	0.108*
C4	0.8109 (3)	0.0965 (3)	0.54406 (11)	0.0698 (9)
H4	0.8512	0.0863	0.5176	0.084*
C5	0.7678 (3)	0.2102 (2)	0.55580 (9)	0.0534 (6)
C6	0.7810 (2)	0.3201 (2)	0.52706 (8)	0.0463 (5)
C7	0.8646 (2)	0.3213 (2)	0.49286 (8)	0.0487 (6)
H7	0.9159	0.2530	0.4880	0.058*
C8	0.8716 (2)	0.4248 (2)	0.46597 (7)	0.0412 (5)
C9	0.7944 (2)	0.5249 (2)	0.47579 (8)	0.0459 (5)
H9	0.7971	0.5964	0.4590	0.055*
C10	0.7135 (2)	0.5180 (2)	0.51051 (8)	0.0432 (5)
C11	0.6290 (2)	0.6236 (2)	0.52240 (8)	0.0472 (6)
C12	0.6129 (3)	0.7268 (3)	0.49576 (11)	0.0631 (7)
H12	0.6549	0.7329	0.4695	0.076*
C13	0.5341 (3)	0.8211 (3)	0.50828 (13)	0.0785 (9)
H13	0.5232	0.8918	0.4909	0.094*
C14	0.4719 (3)	0.8092 (3)	0.54682 (13)	0.0810 (10)
H14	0.4186	0.8714	0.5563	0.097*
C15	0.4906 (3)	0.7035 (3)	0.57070 (12)	0.0805 (10)
H15	0.4477	0.6950	0.5966	0.097*
C16	0.9562 (2)	0.4271 (2)	0.42791 (8)	0.0442 (5)
C17	1.0168 (4)	0.3227 (3)	0.41471 (11)	0.0782 (10)
H17	1.0084	0.2507	0.4307	0.094*
C18	1.0903 (4)	0.3227 (3)	0.37802 (12)	0.0806 (10)
H18	1.1317	0.2510	0.3703	0.097*
C19	1.1035 (3)	0.4254 (3)	0.35296 (9)	0.0544 (6)
C20	1.0478 (3)	0.5310 (3)	0.36688 (10)	0.0680 (8)
H20	1.0580	0.6030	0.3510	0.082*
C21	0.9763 (3)	0.5325 (3)	0.40425 (10)	0.0601 (7)
H21	0.9415	0.6059	0.4134	0.072*
C22	1.1736 (3)	0.4222 (3)	0.31074 (10)	0.0654 (8)
H22A	1.1898	0.3384	0.3023	0.078*
H22B	1.1186	0.4611	0.2857	0.078*
C23	0.6229 (3)	0.5043 (3)	0.71396 (8)	0.0558 (7)
C24	0.6558 (4)	0.5487 (3)	0.75690 (10)	0.0733 (9)
H24	0.7364	0.5895	0.7645	0.088*
C25	0.5659 (4)	0.5321 (4)	0.78984 (11)	0.0891 (11)

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H25	0.5892	0.5605	0.8192	0.107*
C26	0.4473 (4)	0.4757 (4)	0.77919 (11)	0.0804 (10)
H26	0.3892	0.4669	0.8012	0.097*
C27	0.4105 (3)	0.4299 (3)	0.73521 (10)	0.0609 (7)
C28	0.2875 (3)	0.3705 (3)	0.72234 (11)	0.0717 (9)
H28	0.2256	0.3621	0.7431	0.086*
C29	0.2598 (3)	0.3259 (3)	0.67989 (12)	0.0744 (9)
H29	0.1796	0.2853	0.6713	0.089*
C30	0.3534 (3)	0.3414 (3)	0.64886 (10)	0.0710 (8)
H30	0.3333	0.3094	0.6198	0.085*
C31	0.4993 (3)	0.4438 (2)	0.70169 (9)	0.0511 (6)
C32	0.1542 (7)	0.7098 (6)	0.7540 (3)	0.163 (2)
H32A	0.0821	0.7381	0.7698	0.244*
H32B	0.2378	0.7227	0.7726	0.244*
H32C	0.1429	0.6243	0.7475	0.244*
C33	0.2519 (5)	0.7433 (6)	0.6824 (2)	0.160 (3)
H33A	0.2429	0.7970	0.6566	0.241*
H33B	0.2373	0.6606	0.6723	0.241*
H33C	0.3403	0.7509	0.6983	0.241*
C34	0.0645 (5)	0.8613 (4)	0.70234 (18)	0.1072 (14)
H34	0.0688	0.9030	0.6752	0.129*
Cl1	0.17980 (9)	0.06784 (7)	0.58331 (3)	0.0737 (2)
N1	0.7077 (3)	0.2271 (2)	0.59336 (8)	0.0769 (8)
N2	0.7070 (2)	0.41714 (18)	0.53544 (7)	0.0451 (5)
N3	0.5667 (3)	0.6108 (2)	0.55944 (8)	0.0645 (6)
N4	0.4683 (2)	0.3990 (2)	0.65858 (7)	0.0567 (6)
N5	0.1541 (4)	0.7757 (4)	0.71246 (16)	0.1093 (11)
O1	0.70259 (19)	0.5143 (2)	0.67959 (6)	0.0649 (5)
O2	0.3231 (3)	0.0703 (3)	0.58888 (11)	0.1059 (9)
O3	0.1299 (4)	-0.0427 (3)	0.56646 (13)	0.1260 (12)
O4	0.1325 (5)	0.0871 (4)	0.62572 (16)	0.180 (2)
O5	0.1337 (3)	0.1632 (3)	0.55563 (17)	0.1655 (18)
O6	-0.0233 (4)	0.8916 (3)	0.72468 (14)	0.1380 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.08213 (18)	0.08620 (19)	0.04559 (13)	-0.00483 (12)	0.03491 (11)	-0.00590 (10)
C1	0.160 (4)	0.082 (2)	0.082 (2)	0.015 (3)	0.077 (3)	0.026 (2)
C2	0.158 (4)	0.078 (3)	0.100 (3)	0.021 (3)	0.076 (3)	0.040 (2)
C3	0.107 (3)	0.068 (2)	0.106 (3)	0.0214 (19)	0.055 (2)	0.028 (2)
C4	0.081 (2)	0.0640 (19)	0.0718 (19)	0.0146 (15)	0.0415 (17)	0.0185 (14)
C5	0.0590 (15)	0.0576 (16)	0.0474 (14)	0.0007 (12)	0.0221 (12)	0.0081 (12)
C6	0.0492 (13)	0.0519 (14)	0.0403 (12)	-0.0003 (11)	0.0156 (10)	0.0025 (10)
C7	0.0544 (14)	0.0475 (14)	0.0483 (13)	0.0059 (11)	0.0227 (11)	0.0026 (11)
C8	0.0407 (12)	0.0509 (13)	0.0337 (11)	-0.0011 (10)	0.0109 (9)	-0.0006 (9)
C9	0.0505 (14)	0.0482 (13)	0.0409 (12)	0.0029 (11)	0.0134 (10)	0.0034 (10)
C10	0.0427 (13)	0.0500 (14)	0.0383 (12)	-0.0016 (10)	0.0108 (10)	-0.0037 (10)

C11	0.0426 (13)	0.0541 (14)	0.0464 (13)	-0.0006 (11)	0.0120 (10)	-0.0076 (11)
C12	0.0659 (17)	0.0560 (17)	0.0712 (18)	0.0059 (14)	0.0245 (14)	-0.0010 (14)
C13	0.082 (2)	0.0589 (19)	0.100 (3)	0.0136 (16)	0.0305 (19)	-0.0012 (17)
C14	0.077 (2)	0.074 (2)	0.097 (3)	0.0214 (18)	0.0289 (19)	-0.0159 (19)
C15	0.081 (2)	0.092 (3)	0.076 (2)	0.0163 (19)	0.0429 (17)	-0.0136 (19)
C16	0.0448 (12)	0.0531 (14)	0.0370 (11)	0.0004 (11)	0.0143 (10)	-0.0004 (10)
C17	0.110 (3)	0.0582 (18)	0.078 (2)	0.0189 (17)	0.0595 (19)	0.0140 (15)
C18	0.111 (3)	0.0619 (19)	0.081 (2)	0.0178 (18)	0.062 (2)	0.0014 (16)
C19	0.0544 (15)	0.0674 (17)	0.0453 (13)	-0.0058 (13)	0.0220 (11)	-0.0067 (12)
C20	0.082 (2)	0.0683 (18)	0.0608 (17)	0.0028 (16)	0.0380 (16)	0.0150 (14)
C21	0.0707 (18)	0.0545 (15)	0.0611 (16)	0.0067 (13)	0.0331 (14)	0.0062 (13)
C22	0.0670 (18)	0.084 (2)	0.0498 (15)	-0.0139 (15)	0.0280 (13)	-0.0125 (14)
C23	0.0615 (16)	0.0705 (18)	0.0409 (13)	0.0039 (13)	0.0286 (12)	-0.0040 (12)
C24	0.081 (2)	0.094 (2)	0.0510 (16)	-0.0151 (17)	0.0307 (15)	-0.0187 (15)
C25	0.103 (3)	0.122 (3)	0.0496 (17)	-0.020 (2)	0.0410 (18)	-0.0262 (18)
C26	0.092 (2)	0.103 (3)	0.0559 (17)	-0.009 (2)	0.0482 (17)	-0.0122 (17)
C27	0.0656 (17)	0.0709 (18)	0.0523 (15)	0.0054 (14)	0.0329 (13)	0.0022 (13)
C28	0.070 (2)	0.083 (2)	0.069 (2)	0.0011 (16)	0.0406 (16)	0.0095 (17)
C29	0.0655 (19)	0.089 (2)	0.071 (2)	-0.0088 (17)	0.0203 (15)	0.0065 (17)
C30	0.072 (2)	0.094 (2)	0.0502 (16)	-0.0101 (17)	0.0173 (14)	-0.0025 (15)
C31	0.0598 (16)	0.0558 (15)	0.0426 (13)	0.0086 (12)	0.0269 (12)	0.0015 (10)
C32	0.172 (6)	0.138 (5)	0.174 (6)	0.005 (4)	0.000 (5)	0.008 (5)
C33	0.113 (4)	0.151 (5)	0.228 (7)	0.012 (4)	0.065 (4)	-0.052 (5)
C34	0.103 (3)	0.095 (3)	0.132 (4)	-0.008 (3)	0.045 (3)	-0.008 (3)
Cl1	0.0887 (6)	0.0615 (5)	0.0756 (5)	-0.0031 (4)	0.0286 (4)	-0.0032 (4)
N1	0.108 (2)	0.0706 (17)	0.0612 (15)	0.0056 (15)	0.0482 (15)	0.0132 (12)
N2	0.0458 (11)	0.0533 (12)	0.0384 (10)	-0.0010 (9)	0.0137 (8)	0.0005 (9)
N3	0.0684 (15)	0.0729 (16)	0.0570 (14)	0.0133 (12)	0.0274 (12)	-0.0021 (12)
N4	0.0608 (14)	0.0696 (15)	0.0431 (11)	-0.0014 (11)	0.0212 (10)	0.0008 (10)
N5	0.099 (3)	0.094 (3)	0.138 (3)	-0.003 (2)	0.024 (2)	-0.016 (2)
O1	0.0634 (12)	0.0923 (15)	0.0450 (10)	-0.0149 (10)	0.0314 (9)	-0.0126 (10)
O2	0.0906 (19)	0.113 (2)	0.115 (2)	0.0127 (15)	0.0156 (16)	0.0025 (16)
O3	0.158 (3)	0.0764 (18)	0.151 (3)	-0.0307 (19)	0.051 (2)	-0.0370 (19)
O4	0.185 (4)	0.239 (5)	0.130 (3)	-0.052 (3)	0.081 (3)	-0.081 (3)
O5	0.091 (2)	0.121 (3)	0.284 (5)	0.0051 (19)	0.021 (3)	0.105 (3)
O6	0.125 (3)	0.140 (3)	0.165 (3)	0.011 (2)	0.082 (2)	-0.011 (2)

Geometric parameters (Å, °)

Ag1—O1	2.5995 (19)	C19—C20	1.370 (4)
Ag1—N1	2.434 (3)	C19—C22	1.508 (3)
Ag1—N2	2.3572 (19)	C20—C21	1.390 (4)
Ag1—N3	2.414 (3)	C20—H20	0.9300
Ag1—N4	2.275 (2)	C21—H21	0.9300
C1—N1	1.338 (4)	C22—O1 ⁱ	1.426 (3)
C1—C2	1.361 (5)	C22—H22A	0.9700
C1—H1	0.9300	C22—H22B	0.9700
C2—C3	1.363 (5)	C23—C24	1.367 (4)
C2—H2	0.9300	C23—O1	1.373 (3)

supplementary materials

C3—C4	1.382 (4)	C23—C31	1.418 (4)
C3—H3	0.9300	C24—C25	1.419 (4)
C4—C5	1.377 (4)	C24—H24	0.9300
C4—H4	0.9300	C25—C26	1.347 (5)
C5—N1	1.341 (3)	C25—H25	0.9300
C5—C6	1.489 (3)	C26—C27	1.406 (4)
C6—N2	1.338 (3)	C26—H26	0.9300
C6—C7	1.392 (3)	C27—C28	1.410 (5)
C7—C8	1.392 (3)	C27—C31	1.421 (3)
C7—H7	0.9300	C28—C29	1.348 (5)
C8—C9	1.395 (3)	C28—H28	0.9300
C8—C16	1.491 (3)	C29—C30	1.402 (4)
C9—C10	1.387 (3)	C29—H29	0.9300
C9—H9	0.9300	C30—N4	1.318 (4)
C10—N2	1.335 (3)	C30—H30	0.9300
C10—C11	1.501 (3)	C31—N4	1.371 (3)
C11—N3	1.335 (3)	C32—N5	1.428 (7)
C11—C12	1.378 (4)	C32—H32A	0.9600
C12—C13	1.380 (4)	C32—H32B	0.9600
C12—H12	0.9300	C32—H32C	0.9600
C13—C14	1.372 (5)	C33—N5	1.448 (6)
C13—H13	0.9300	C33—H33A	0.9600
C14—C15	1.359 (5)	C33—H33B	0.9600
C14—H14	0.9300	C33—H33C	0.9600
C15—N3	1.337 (4)	C34—O6	1.211 (5)
C15—H15	0.9300	C34—N5	1.310 (6)
C16—C17	1.374 (4)	C34—H34	0.9300
C16—C21	1.379 (4)	Cl1—O5	1.375 (3)
C17—C18	1.385 (4)	Cl1—O3	1.382 (3)
C17—H17	0.9300	Cl1—O4	1.412 (4)
C18—C19	1.363 (4)	Cl1—O2	1.432 (3)
C18—H18	0.9300	O1—C22 ⁱ	1.426 (4)
N4—Ag1—N2	167.56 (8)	O1 ⁱ —C22—C19	107.7 (2)
N4—Ag1—N3	115.30 (8)	O1 ⁱ —C22—H22A	110.2
N2—Ag1—N3	68.62 (7)	C19—C22—H22A	110.2
N4—Ag1—N1	106.16 (8)	O1 ⁱ —C22—H22B	110.2
N2—Ag1—N1	68.55 (7)	C19—C22—H22B	110.2
N3—Ag1—N1	137.12 (7)	H22A—C22—H22B	108.5
N4—Ag1—O1	66.35 (7)	C24—C23—O1	124.4 (3)
N2—Ag1—O1	125.64 (6)	C24—C23—C31	120.9 (2)
N3—Ag1—O1	98.95 (8)	O1—C23—C31	114.7 (2)
N1—Ag1—O1	107.45 (9)	C23—C24—C25	119.5 (3)
N1—C1—C2	123.4 (3)	C23—C24—H24	120.3
N1—C1—H1	118.3	C25—C24—H24	120.3
C2—C1—H1	118.3	C26—C25—C24	121.1 (3)
C1—C2—C3	118.9 (3)	C26—C25—H25	119.5
C1—C2—H2	120.5	C24—C25—H25	119.5
C3—C2—H2	120.5	C25—C26—C27	120.7 (3)

C2—C3—C4	118.7 (3)	C25—C26—H26	119.7
C2—C3—H3	120.7	C27—C26—H26	119.7
C4—C3—H3	120.7	C26—C27—C28	122.9 (3)
C5—C4—C3	119.6 (3)	C26—C27—C31	119.5 (3)
C5—C4—H4	120.2	C28—C27—C31	117.6 (3)
C3—C4—H4	120.2	C29—C28—C27	119.9 (3)
N1—C5—C4	121.4 (2)	C29—C28—H28	120.1
N1—C5—C6	116.3 (2)	C27—C28—H28	120.1
C4—C5—C6	122.3 (2)	C28—C29—C30	119.2 (3)
N2—C6—C7	121.6 (2)	C28—C29—H29	120.4
N2—C6—C5	116.5 (2)	C30—C29—H29	120.4
C7—C6—C5	121.8 (2)	N4—C30—C29	123.6 (3)
C6—C7—C8	120.1 (2)	N4—C30—H30	118.2
C6—C7—H7	120.0	C29—C30—H30	118.2
C8—C7—H7	120.0	N4—C31—C23	120.2 (2)
C7—C8—C9	117.0 (2)	N4—C31—C27	121.5 (3)
C7—C8—C16	121.3 (2)	C23—C31—C27	118.3 (2)
C9—C8—C16	121.7 (2)	N5—C32—H32A	109.5
C10—C9—C8	120.1 (2)	N5—C32—H32B	109.5
C10—C9—H9	119.9	H32A—C32—H32B	109.5
C8—C9—H9	119.9	N5—C32—H32C	109.5
N2—C10—C9	121.8 (2)	H32A—C32—H32C	109.5
N2—C10—C11	116.2 (2)	H32B—C32—H32C	109.5
C9—C10—C11	122.0 (2)	N5—C33—H33A	109.5
N3—C11—C12	121.5 (2)	N5—C33—H33B	109.5
N3—C11—C10	116.5 (2)	H33A—C33—H33B	109.5
C12—C11—C10	122.0 (2)	N5—C33—H33C	109.5
C11—C12—C13	119.5 (3)	H33A—C33—H33C	109.5
C11—C12—H12	120.2	H33B—C33—H33C	109.5
C13—C12—H12	120.2	O6—C34—N5	126.6 (5)
C14—C13—C12	119.1 (3)	O6—C34—H34	116.7
C14—C13—H13	120.5	N5—C34—H34	116.7
C12—C13—H13	120.5	O5—C11—O3	111.6 (3)
C15—C14—C13	117.8 (3)	O5—C11—O4	107.0 (3)
C15—C14—H14	121.1	O3—C11—O4	107.9 (2)
C13—C14—H14	121.1	O5—C11—O2	108.57 (19)
N3—C15—C14	124.4 (3)	O3—C11—O2	112.1 (2)
N3—C15—H15	117.8	O4—C11—O2	109.6 (2)
C14—C15—H15	117.8	C1—N1—C5	117.9 (3)
C17—C16—C21	117.1 (2)	C1—N1—Ag1	123.7 (2)
C17—C16—C8	120.9 (2)	C5—N1—Ag1	117.28 (18)
C21—C16—C8	122.0 (2)	C10—N2—C6	119.36 (19)
C16—C17—C18	121.3 (3)	C10—N2—Ag1	119.76 (15)
C16—C17—H17	119.3	C6—N2—Ag1	119.77 (15)
C18—C17—H17	119.3	C11—N3—C15	117.7 (3)
C19—C18—C17	121.6 (3)	C11—N3—Ag1	117.99 (18)
C19—C18—H18	119.2	C15—N3—Ag1	124.3 (2)
C17—C18—H18	119.2	C30—N4—C31	118.2 (2)
C18—C19—C20	117.6 (2)	C30—N4—Ag1	118.02 (19)

supplementary materials

C18—C19—C22	121.2 (3)	C31—N4—Ag1	123.75 (18)
C20—C19—C22	121.2 (3)	C34—N5—C32	119.4 (5)
C19—C20—C21	121.2 (3)	C34—N5—C33	122.2 (5)
C19—C20—H20	119.4	C32—N5—C33	118.4 (5)
C21—C20—H20	119.4	C23—O1—C22 ⁱ	117.5 (2)
C16—C21—C20	121.1 (3)	C23—O1—Ag1	114.95 (16)
C16—C21—H21	119.5	C22 ⁱ —O1—Ag1	127.44 (14)
C20—C21—H21	119.5		
N1—C1—C2—C3	-2.1 (8)	N4—Ag1—N1—C1	-1.9 (4)
C1—C2—C3—C4	0.6 (7)	N2—Ag1—N1—C1	-170.0 (4)
C2—C3—C4—C5	0.8 (6)	N3—Ag1—N1—C1	-166.9 (3)
C3—C4—C5—N1	-1.0 (5)	O1—Ag1—N1—C1	67.8 (4)
C3—C4—C5—C6	-178.9 (3)	N4—Ag1—N1—C5	165.8 (2)
N1—C5—C6—N2	-14.4 (4)	N2—Ag1—N1—C5	-2.3 (2)
C4—C5—C6—N2	163.7 (3)	N3—Ag1—N1—C5	0.9 (3)
N1—C5—C6—C7	166.4 (3)	O1—Ag1—N1—C5	-124.5 (2)
C4—C5—C6—C7	-15.5 (4)	C9—C10—N2—C6	0.5 (4)
N2—C6—C7—C8	-0.8 (4)	C11—C10—N2—C6	-179.2 (2)
C5—C6—C7—C8	178.4 (2)	C9—C10—N2—Ag1	168.45 (18)
C6—C7—C8—C9	1.4 (4)	C11—C10—N2—Ag1	-11.2 (3)
C6—C7—C8—C16	-177.6 (2)	C7—C6—N2—C10	-0.2 (4)
C7—C8—C9—C10	-1.1 (4)	C5—C6—N2—C10	-179.4 (2)
C16—C8—C9—C10	177.9 (2)	C7—C6—N2—Ag1	-168.13 (19)
C8—C9—C10—N2	0.2 (4)	C5—C6—N2—Ag1	12.7 (3)
C8—C9—C10—C11	179.8 (2)	N4—Ag1—N2—C10	119.3 (4)
N2—C10—C11—N3	6.6 (3)	N3—Ag1—N2—C10	8.49 (18)
C9—C10—C11—N3	-173.0 (2)	N1—Ag1—N2—C10	-173.8 (2)
N2—C10—C11—C12	-171.3 (2)	O1—Ag1—N2—C10	-77.2 (2)
C9—C10—C11—C12	9.0 (4)	N4—Ag1—N2—C6	-72.7 (4)
N3—C11—C12—C13	2.1 (5)	N3—Ag1—N2—C6	176.4 (2)
C10—C11—C12—C13	180.0 (3)	N1—Ag1—N2—C6	-5.86 (18)
C11—C12—C13—C14	-0.8 (5)	O1—Ag1—N2—C6	90.73 (19)
C12—C13—C14—C15	-0.5 (6)	C12—C11—N3—C15	-1.9 (4)
C13—C14—C15—N3	0.7 (6)	C10—C11—N3—C15	-179.9 (3)
C7—C8—C16—C17	8.0 (4)	C12—C11—N3—Ag1	178.9 (2)
C9—C8—C16—C17	-170.9 (3)	C10—C11—N3—Ag1	0.9 (3)
C7—C8—C16—C21	-172.5 (3)	C14—C15—N3—C11	0.5 (5)
C9—C8—C16—C21	8.6 (4)	C14—C15—N3—Ag1	179.7 (3)
C21—C16—C17—C18	-2.6 (5)	N4—Ag1—N3—C11	-171.7 (2)
C8—C16—C17—C18	176.9 (3)	N2—Ag1—N3—C11	-4.6 (2)
C16—C17—C18—C19	-1.3 (6)	N1—Ag1—N3—C11	-7.7 (3)
C17—C18—C19—C20	3.7 (6)	O1—Ag1—N3—C11	120.3 (2)
C17—C18—C19—C22	-174.7 (3)	N4—Ag1—N3—C15	9.1 (3)
C18—C19—C20—C21	-2.3 (5)	N2—Ag1—N3—C15	176.3 (3)
C22—C19—C20—C21	176.2 (3)	N1—Ag1—N3—C15	173.1 (3)
C17—C16—C21—C20	4.0 (5)	O1—Ag1—N3—C15	-58.9 (3)
C8—C16—C21—C20	-175.5 (3)	C29—C30—N4—C31	1.5 (5)
C19—C20—C21—C16	-1.6 (5)	C29—C30—N4—Ag1	-176.6 (3)

C18—C19—C22—O1 ⁱ	-109.7 (3)	C23—C31—N4—C30	178.8 (3)
C20—C19—C22—O1 ⁱ	72.0 (4)	C27—C31—N4—C30	-0.4 (4)
O1—C23—C24—C25	-179.4 (3)	C23—C31—N4—Ag1	-3.3 (3)
C31—C23—C24—C25	1.1 (5)	C27—C31—N4—Ag1	177.55 (19)
C23—C24—C25—C26	-1.5 (6)	N2—Ag1—N4—C30	-14.0 (5)
C24—C25—C26—C27	1.1 (6)	N3—Ag1—N4—C30	91.7 (2)
C25—C26—C27—C28	-179.8 (4)	N1—Ag1—N4—C30	-77.0 (2)
C25—C26—C27—C31	-0.2 (5)	O1—Ag1—N4—C30	-179.3 (3)
C26—C27—C28—C29	-178.3 (3)	N2—Ag1—N4—C31	168.1 (3)
C31—C27—C28—C29	2.1 (5)	N3—Ag1—N4—C31	-86.2 (2)
C27—C28—C29—C30	-1.2 (5)	N1—Ag1—N4—C31	105.0 (2)
C28—C29—C30—N4	-0.7 (6)	O1—Ag1—N4—C31	2.70 (19)
C24—C23—C31—N4	-179.5 (3)	O6—C34—N5—C32	-1.1 (8)
O1—C23—C31—N4	1.0 (4)	O6—C34—N5—C33	177.5 (5)
C24—C23—C31—C27	-0.3 (4)	C24—C23—O1—C22 ⁱ	-1.6 (4)
O1—C23—C31—C27	-179.8 (2)	C31—C23—O1—C22 ⁱ	178.0 (3)
C26—C27—C31—N4	179.0 (3)	C24—C23—O1—Ag1	-178.2 (3)
C28—C27—C31—N4	-1.3 (4)	C31—C23—O1—Ag1	1.3 (3)
C26—C27—C31—C23	-0.2 (4)	N4—Ag1—O1—C23	-2.03 (18)
C28—C27—C31—C23	179.4 (3)	N2—Ag1—O1—C23	-178.19 (17)
C2—C1—N1—C5	2.0 (7)	N3—Ag1—O1—C23	111.75 (19)
C2—C1—N1—Ag1	169.7 (4)	N1—Ag1—O1—C23	-102.4 (2)
C4—C5—N1—C1	-0.4 (5)	N4—Ag1—O1—C22 ⁱ	-178.3 (3)
C6—C5—N1—C1	177.7 (3)	N2—Ag1—O1—C22 ⁱ	5.5 (3)
C4—C5—N1—Ag1	-168.9 (2)	N3—Ag1—O1—C22 ⁱ	-64.5 (2)
C6—C5—N1—Ag1	9.2 (3)	N1—Ag1—O1—C22 ⁱ	81.3 (3)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C4—H4 \cdots O3 ⁱⁱ	0.93	2.57	3.450 (5)	158
C12—H12 \cdots O5 ⁱⁱⁱ	0.93	2.60	3.344 (5)	138
C28—H28 \cdots O6 ^{iv}	0.93	2.37	3.250 (5)	158
C29—H29 \cdots O4	0.93	2.57	3.252 (6)	130

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

Fig. 1

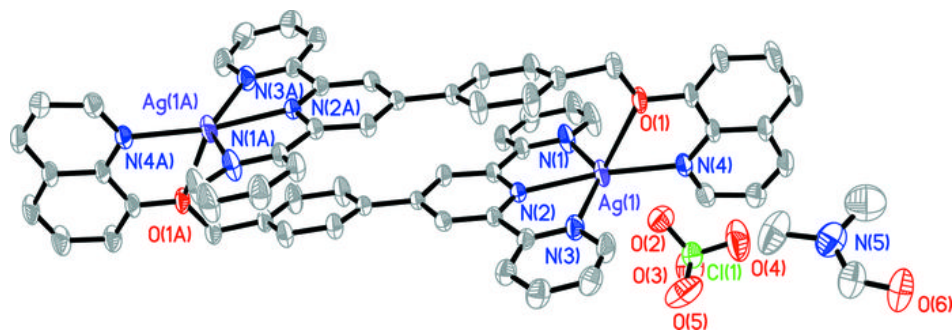


Fig. 2

