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The non-centrosymmetric polymorph of (quinolin-8-ol-κ^2N,O)(quinolin-8-olato-κ^2N,O)silver(I)

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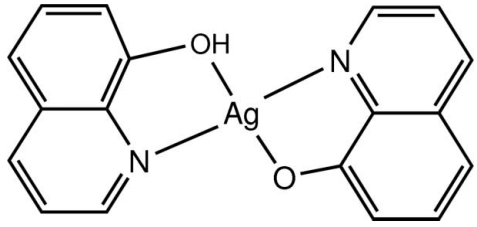
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.057; data-to-parameter ratio = 12.3.

The title compound, [Ag(C_9H_6NO)(C_9H_7NO)], crystallizes as a non-centrosymmetric polymorph. The structure was previously reported by Wu *et al.* [(2006). *Acta Cryst.* E**62**, m281–m282] in the centrosymmetric space group *Pbcn*. The Ag^I ion displays a distorted tetrahedral coordination geometry defined by two N and two O atoms from a neutral quinolin-8-ol ligand (HQ) and a deprotonated quinolin-8-olate anion (Q^-). The dihedral angle between the two ligands is 47.0 (1)°. Strong O—H···O hydrogen bonds link the molecules into a supramolecular chain along the *a*-axis direction.

Related literature

For the centrosymmetric polymorph, see: Wu *et al.* (2006).



Experimental

Crystal data

[Ag(C_9H_6NO)(C_9H_7NO)]
M_r = 397.17
Orthorhombic, $P2_12_12_1$
a = 7.2320 (3) Å
b = 10.4857 (6) Å
c = 18.9398 (10) Å
V = 1436.25 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 293 K
0.19 × 0.18 × 0.15 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.884, T_{max} = 1.000
8103 measured reflections
2554 independent reflections
2305 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.057
S = 1.08
2554 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1056 Friedel pairs
Flack parameter: −0.02 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.73	2.495 (3)	154

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5282).

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Wu, H., Dong, X.-W., Liu, H.-Y. & Ma, J.-F. (2006). *Acta Cryst.* E**62**, m281–m282.

supporting information

Acta Cryst. (2013). E**69**, m133 [doi:10.1107/S160053681300281X]

The non-centrosymmetric polymorph of (quinolin-8-ol-κ^2N,O)(quinolin-8-olato-κ^2N,O)silver(I)

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S1. Comment

In the title compound,(I), the Ag ion is four-coordinated by two nitrogen atoms and two oxygen atoms from two 8-hydroxyquinoline ligands, forming a distorted tetrahedral geometry (Fig. 1). The two 8-hydroxyquinoline ligands are different in their mode of the coordination. One is a neutral ligand while the other is deprotonated. The dihedral angle between two 8-hydroxyquinoline mean planes is 47.0 (1)°. A polymorph (II) of the structure has been previously reported by Wu *et al.* (2006) in the centrosymmetric space group *Pbcn* with *a* = 11.434 (2)Å, *b* = 14.817 (3)Å, *c* = 8.7828 (18)Å. The Ag-N bondlengths of 2.174 (3), 2.176 (3)Å in (I) are shorter than the value of 2.2377 (19)Å for (II) while the Ag-O bondlengths of 2.596 (2), 2.649 (2)Å are longer than the value of 2.4831 (17)Å found for (II). Inter-molecular O_H···O hydrogen bonding between HQ and Q^- ligands form a supramolecular chain structure (Table 1, Fig. 2). Weak π-π interactions are observed between neighboring aromatic rings [dihedral angle 2.0 (2)°] with the centroid-to-centroid distance of 3.75 (1) Å, which is favorable to increase the stability of the structure (Fig. 3).

S2. Experimental

A methanol solution (15 ml) of 8-hydroxyquinoline(HQ) (0.075 g,0.5 mmol) was mixed with an aqueous solution (5 ml) of $AgNO_3$ (0.085 g, 0.5 mmol). Ammonia solution was dropped into the mixture under stirring until it was almost clear. Then it was filtered. Yellow single crystals, suitable for X-ray, were obtained after several days.

S3. Refinement

The H atoms on C atoms and O atom were placed in idealized positions and refined as riding atoms with C—H = 0.93 Å and O—H = 0.84 (2) Å, with U_{iso}(H) = 1.2U_{eq}(C).

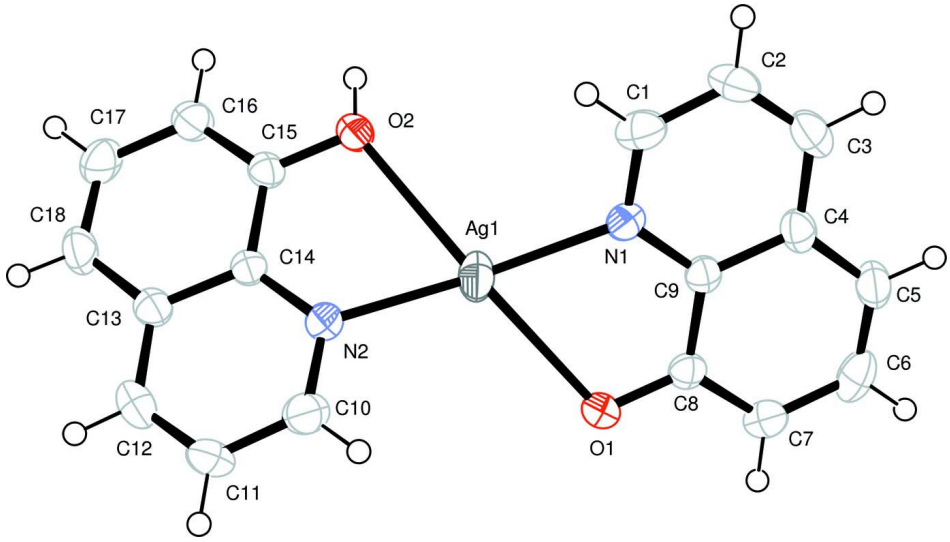

Figure 1

The molecular structure of (I).

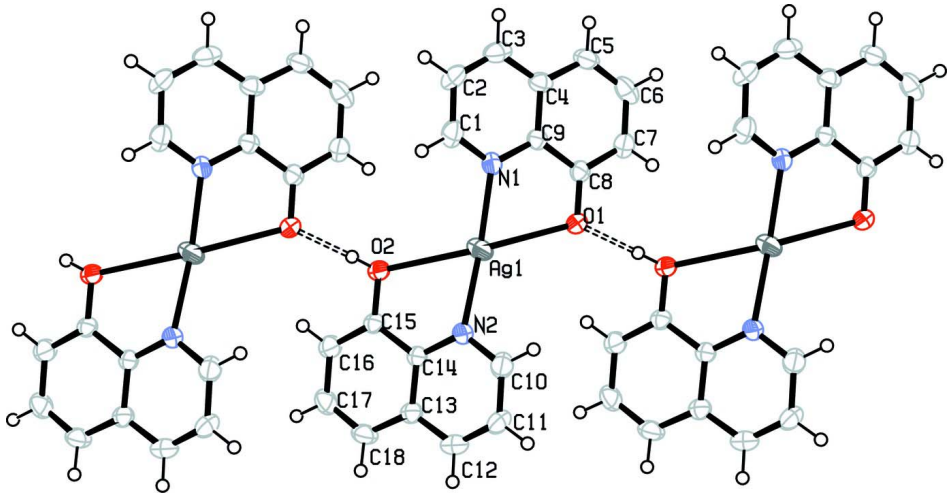

Figure 2

View of the hydrogen-bonding chain of (1). Hydrogen bonds are drawn as dashed lines.

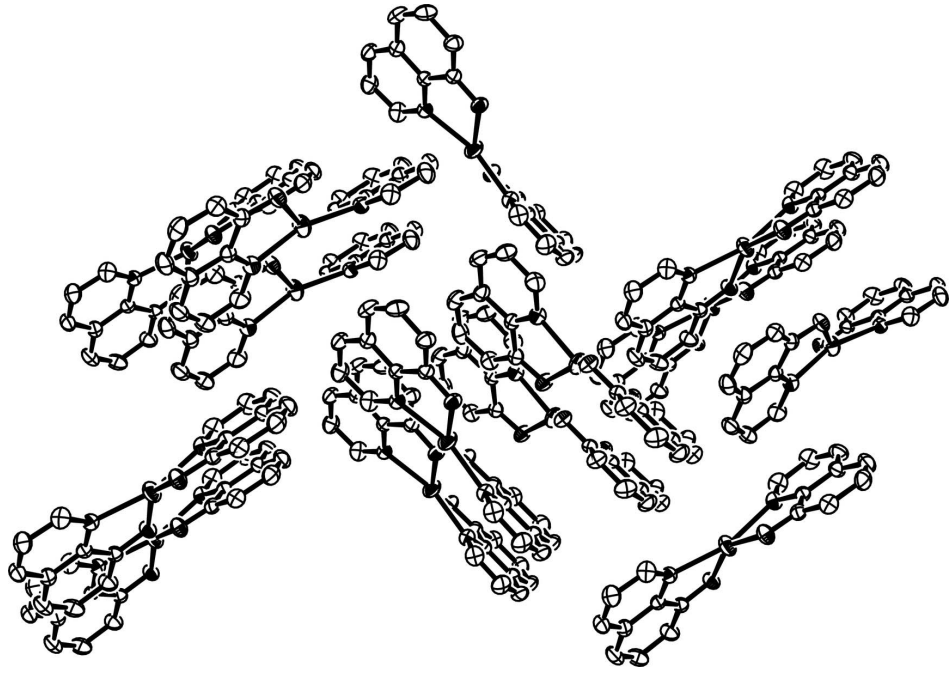

Figure 3

View of the packing. H atoms have been omitted for clarity.

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Crystal data

$[Ag(C_9H_6NO)(C_9H_7NO)]$
$M_r = 397.17$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.2320$ (3) Å
$b = 10.4857$ (6) Å
$c = 18.9398$ (10) Å
$V = 1436.25$ (13) Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.837$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3403 reflections
$\theta = 2.8$–$29.6°$
$\mu = 1.42$ mm^{-1}
$T = 293$ K
Block, yellow
0.19 × 0.18 × 0.15 mm

Data collection

Bruker SMART diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.3592 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.884$, $T_{max} = 1.000$
8103 measured reflections
2554 independent reflections
2305 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.9°$
$h = -8\rightarrow7$
$k = -9\rightarrow12$
$l = -22\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.057$
$S = 1.08$
2554 reflections
208 parameters
0 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.022P)^2 + 0.3181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Absolute structure: Flack (1983), 1056 Friedel pairs
Absolute structure parameter: −0.02 (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_{iso}*/U_{eq}
C17	0.3321 (5)	0.5388 (4)	0.2207 (2)	0.0428 (11)
H17	0.2247	0.4904	0.2240	0.051*
C18	0.4685 (6)	0.5214 (4)	0.2684 (2)	0.0413 (11)
H18	0.4528	0.4635	0.3051	0.050*
Ag1	0.87935 (4)	0.85088 (3)	0.101833 (16)	0.04331 (11)
C6	1.4013 (5)	1.0168 (4)	−0.0955 (2)	0.0428 (10)
H6	1.5083	1.0187	−0.1227	0.051*
O2	0.5261 (3)	0.7849 (2)	0.10618 (14)	0.0319 (6)
H2A	0.4318	0.7863	0.0821	0.048*
O1	1.2184 (3)	0.8451 (3)	0.05683 (12)	0.0347 (6)
C8	1.2323 (5)	0.9235 (4)	0.00265 (19)	0.0279 (8)
C7	1.3899 (6)	0.9315 (4)	−0.03871 (19)	0.0360 (9)
H7	1.4903	0.8791	−0.0286	0.043*
C9	1.0833 (4)	1.0077 (3)	−0.01372 (18)	0.0264 (8)
C13	0.6343 (5)	0.5908 (3)	0.26259 (18)	0.0300 (8)
C15	0.5067 (5)	0.6993 (3)	0.15794 (19)	0.0268 (8)
N1	0.9246 (4)	1.0033 (3)	0.02576 (16)	0.0309 (8)
N2	0.8161 (4)	0.7483 (3)	0.19863 (16)	0.0280 (7)
C11	0.9365 (5)	0.6477 (5)	0.3027 (2)	0.0406 (10)
H11	1.0325	0.6407	0.3352	0.049*
C16	0.3498 (5)	0.6289 (4)	0.1662 (2)	0.0372 (9)
H16	0.2520	0.6408	0.1350	0.045*
C14	0.6564 (4)	0.6808 (3)	0.20672 (18)	0.0245 (8)
C2	0.7975 (5)	1.1738 (4)	−0.0422 (2)	0.0435 (11)
H2	0.6996	1.2297	−0.0497	0.052*
C4	1.0976 (5)	1.0959 (3)	−0.07134 (19)	0.0325 (9)
C3	0.9487 (6)	1.1781 (4)	−0.0839 (2)	0.0411 (11)
H3	0.9540	1.2359	−0.1211	0.049*

C10	0.9497 (5)	0.7328 (4)	0.2455 (2)	0.0404 (10)
H10	1.0574	0.7804	0.2404	0.048*
C1	0.7905 (5)	1.0843 (4)	0.0121 (2)	0.0414 (11)
H1	0.6851	1.0818	0.0402	0.050*
C12	0.7824 (6)	0.5764 (4)	0.3098 (2)	0.0388 (10)
H12	0.7742	0.5172	0.3462	0.047*
C5	1.2597 (5)	1.0971 (4)	−0.1118 (2)	0.0401 (10)
H5	1.2705	1.1526	−0.1498	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C17	0.033 (2)	0.037 (3)	0.059 (3)	−0.0098 (19)	0.0030 (19)	0.007 (2)
C18	0.047 (2)	0.035 (3)	0.042 (3)	0.002 (2)	0.010 (2)	0.015 (2)
Ag1	0.04359 (16)	0.04830 (19)	0.03805 (17)	−0.00869 (17)	0.00683 (17)	0.01115 (17)
C6	0.039 (2)	0.054 (3)	0.036 (2)	−0.013 (2)	0.013 (2)	−0.006 (2)
O2	0.0300 (11)	0.0322 (14)	0.0337 (14)	−0.0030 (11)	−0.0046 (13)	0.0085 (14)
O1	0.0289 (12)	0.0401 (16)	0.0350 (14)	0.0029 (14)	−0.0021 (11)	0.0112 (15)
C8	0.0259 (18)	0.031 (2)	0.027 (2)	−0.0041 (18)	−0.0037 (16)	−0.0017 (18)
C7	0.0288 (18)	0.041 (2)	0.038 (2)	0.002 (2)	−0.002 (2)	−0.0019 (18)
C9	0.0271 (19)	0.027 (2)	0.0249 (19)	−0.0052 (17)	−0.0029 (15)	−0.0009 (15)
C13	0.0324 (18)	0.029 (2)	0.028 (2)	0.008 (2)	0.0037 (18)	0.0008 (15)
C15	0.0291 (18)	0.023 (2)	0.028 (2)	0.0052 (16)	0.0018 (16)	0.0009 (17)
N1	0.0246 (16)	0.0364 (19)	0.0318 (18)	−0.0006 (15)	0.0009 (12)	0.0021 (14)
N2	0.0268 (15)	0.0289 (18)	0.0283 (17)	0.0006 (14)	0.0010 (13)	0.0005 (15)
C11	0.037 (2)	0.049 (3)	0.036 (2)	0.005 (2)	−0.0110 (16)	0.006 (2)
C16	0.034 (2)	0.035 (2)	0.043 (2)	−0.004 (2)	−0.0063 (17)	0.0065 (18)
C14	0.0257 (17)	0.022 (2)	0.0257 (18)	0.0052 (16)	0.0037 (14)	−0.0016 (15)
C2	0.041 (2)	0.042 (3)	0.048 (3)	0.014 (2)	−0.009 (2)	0.007 (2)
C4	0.039 (2)	0.029 (2)	0.029 (2)	−0.008 (2)	−0.0038 (17)	0.0036 (15)
C3	0.053 (2)	0.030 (2)	0.040 (3)	−0.0032 (19)	−0.0094 (19)	0.0092 (19)
C10	0.032 (2)	0.050 (3)	0.040 (2)	0.002 (2)	−0.0016 (18)	0.000 (2)
C1	0.031 (2)	0.049 (3)	0.044 (3)	0.008 (2)	0.0000 (19)	−0.003 (2)
C12	0.051 (2)	0.034 (3)	0.030 (2)	0.003 (2)	0.0009 (19)	0.0078 (19)
C5	0.044 (2)	0.041 (3)	0.035 (2)	−0.010 (2)	0.001 (2)	0.011 (2)

Geometric parameters (Å, º)

C17—C18	1.349 (6)	C13—C14	1.427 (5)
C17—C16	1.406 (5)	C15—C16	1.362 (5)
C17—H17	0.9300	C15—C14	1.436 (5)
C18—C13	1.407 (6)	N1—C1	1.316 (5)
C18—H18	0.9300	N2—C10	1.322 (5)
Ag1—N2	2.174 (3)	N2—C14	1.364 (4)
Ag1—N1	2.176 (3)	C11—C12	1.348 (5)
Ag1—O1	2.596 (2)	C11—C10	1.408 (6)
Ag1—O2	2.649 (2)	C11—H11	0.9300
C6—C5	1.361 (6)	C16—H16	0.9300

C6—C7	1.401 (5)	C2—C3	1.349 (5)
C6—H6	0.9300	C2—C1	1.394 (6)
O2—C15	1.336 (4)	C2—H2	0.9300
O2—H2A	0.8200	C4—C3	1.400 (5)
O1—C8	1.319 (4)	C4—C5	1.400 (6)
C8—C7	1.386 (5)	C3—H3	0.9300
C8—C9	1.427 (5)	C10—H10	0.9300
C7—H7	0.9300	C1—H1	0.9300
C9—N1	1.370 (4)	C12—H12	0.9300
C9—C4	1.434 (5)	C5—H5	0.9300
C13—C12	1.403 (5)		

C18—C17—C16	121.1 (4)	C9—N1—Ag1	120.8 (2)
C18—C17—H17	119.5	C10—N2—C14	118.7 (3)
C16—C17—H17	119.5	C10—N2—Ag1	118.3 (2)
C17—C18—C13	120.1 (4)	C14—N2—Ag1	122.0 (2)
C17—C18—H18	120.0	C12—C11—C10	118.9 (3)
C13—C18—H18	120.0	C12—C11—H11	120.5
N2—Ag1—N1	162.38 (12)	C10—C11—H11	120.5
N2—Ag1—O1	117.62 (9)	C15—C16—C17	121.6 (3)
N1—Ag1—O1	70.00 (10)	C15—C16—H16	119.2
N2—Ag1—O2	69.00 (9)	C17—C16—H16	119.2
N1—Ag1—O2	110.96 (9)	N2—C14—C13	121.4 (3)
O1—Ag1—O2	156.21 (9)	N2—C14—C15	119.7 (3)
C5—C6—C7	121.7 (4)	C13—C14—C15	118.8 (3)
C5—C6—H6	119.2	C3—C2—C1	118.9 (4)
C7—C6—H6	119.2	C3—C2—H2	120.5
C15—O2—H2A	109.5	C1—C2—H2	120.5
C8—O1—Ag1	108.2 (2)	C3—C4—C5	123.0 (4)
O1—C8—C7	122.7 (3)	C3—C4—C9	118.1 (4)
O1—C8—C9	119.8 (3)	C5—C4—C9	118.8 (3)
C7—C8—C9	117.4 (3)	C2—C3—C4	120.2 (4)
C8—C7—C6	121.4 (4)	C2—C3—H3	119.9
C8—C7—H7	119.3	C4—C3—H3	119.9
C6—C7—H7	119.3	N2—C10—C11	123.1 (4)
N1—C9—C8	119.5 (3)	N2—C10—H10	118.5
N1—C9—C4	119.8 (3)	C11—C10—H10	118.5
C8—C9—C4	120.6 (3)	N1—C1—C2	123.6 (4)
C12—C13—C18	123.1 (3)	N1—C1—H1	118.2
C12—C13—C14	117.3 (4)	C2—C1—H1	118.2
C18—C13—C14	119.7 (3)	C11—C12—C13	120.5 (4)
O2—C15—C16	122.3 (3)	C11—C12—H12	119.7
O2—C15—C14	118.9 (3)	C13—C12—H12	119.7
C16—C15—C14	118.8 (3)	C6—C5—C4	120.0 (4)
C1—N1—C9	119.2 (3)	C6—C5—H5	120.0
C1—N1—Ag1	119.6 (3)	C4—C5—H5	120.0

C16—C17—C18—C13	−2.2 (7)	Ag1—N2—C14—C13	165.2 (2)

N2—Ag1—O1—C8	−173.2 (2)	C10—N2—C14—C15	177.8 (3)
N1—Ag1—O1—C8	−10.6 (2)	Ag1—N2—C14—C15	−14.3 (4)
Ag1—O1—C8—C7	−172.3 (3)	C12—C13—C14—N2	1.3 (5)
Ag1—O1—C8—C9	9.9 (4)	C18—C13—C14—N2	−178.9 (3)
O1—C8—C7—C6	−179.3 (4)	C12—C13—C14—C15	−179.2 (3)
C9—C8—C7—C6	−1.4 (5)	C18—C13—C14—C15	0.6 (5)
C5—C6—C7—C8	1.1 (6)	O2—C15—C14—N2	−1.4 (5)
O1—C8—C9—N1	−2.1 (5)	C16—C15—C14—N2	178.7 (3)
C7—C8—C9—N1	−180.0 (3)	O2—C15—C14—C13	179.1 (3)
O1—C8—C9—C4	178.4 (3)	C16—C15—C14—C13	−0.9 (5)
C7—C8—C9—C4	0.5 (5)	N1—C9—C4—C3	1.9 (5)
C17—C18—C13—C12	−179.3 (4)	C8—C9—C4—C3	−178.6 (3)
C17—C18—C13—C14	0.9 (6)	N1—C9—C4—C5	−178.8 (3)
C8—C9—N1—C1	177.5 (3)	C8—C9—C4—C5	0.7 (5)
C4—C9—N1—C1	−3.0 (5)	C1—C2—C3—C4	−1.6 (6)
C8—C9—N1—Ag1	−9.7 (4)	C5—C4—C3—C2	−178.9 (4)
C4—C9—N1—Ag1	169.8 (2)	C9—C4—C3—C2	0.4 (6)
N2—Ag1—N1—C1	−57.9 (5)	C14—N2—C10—C11	1.4 (6)
O1—Ag1—N1—C1	−176.8 (3)	Ag1—N2—C10—C11	−167.0 (3)
N2—Ag1—N1—C9	129.4 (4)	C12—C11—C10—N2	1.3 (6)
O1—Ag1—N1—C9	10.4 (2)	C9—N1—C1—C2	1.8 (6)
N1—Ag1—N2—C10	−84.3 (4)	Ag1—N1—C1—C2	−171.1 (3)
O1—Ag1—N2—C10	27.5 (3)	C3—C2—C1—N1	0.5 (7)
N1—Ag1—N2—C14	107.7 (4)	C10—C11—C12—C13	−2.7 (6)
O1—Ag1—N2—C14	−140.4 (2)	C18—C13—C12—C11	−178.3 (4)
O2—C15—C16—C17	179.7 (4)	C14—C13—C12—C11	1.5 (6)
C14—C15—C16—C17	−0.4 (6)	C7—C6—C5—C4	0.2 (6)
C18—C17—C16—C15	2.0 (7)	C3—C4—C5—C6	178.2 (4)
C10—N2—C14—C13	−2.7 (5)	C9—C4—C5—C6	−1.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1^{i}	0.82	1.73	2.495 (3)	154

Symmetry code: (i) *x*−1, *y*, *z*.