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Bis[μ -2-[(pyrimidin-2-yl)aminomethyl]-phenolato]- $\kappa^2 N^1:O$; $\kappa^2 O:N^1$ -bis[2-[(pyrimidin-2-yl- κN)aminomethyl]phenol]silver(I) dihydrate

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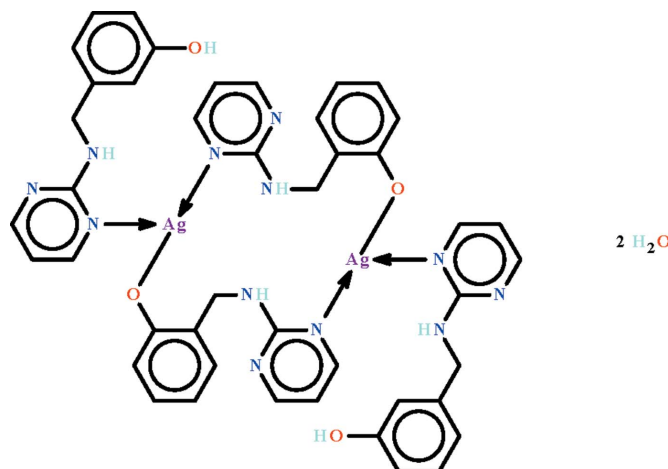
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.044; wR factor = 0.133; data-to-parameter ratio = 16.0.

The Ag^I atom in the title centrosymmetric dinuclear compound, $[Ag_2(C_{11}H_{10}N_3O)_2(C_{11}H_{11}N_3O)_2] \cdot 2H_2O$, shows a T -shaped coordination arising from bonding to the N atom of a neutral 2-[(pyrimidin-2-yl)aminomethyl]phenol ligand, the N atom of the 2-[(pyrimidin-2-yl)aminomethyl]phenolate anion [$N-Ag-N = 171.8(1)^\circ$] and the terminal O atom of the other anion [$Ag-O = 2.606(3)$ Å]. A pair of 2-[(pyrimidin-2-yl)aminomethyl]phenolate anions link the two Ag^I atoms to form the dinuclear compound. In the crystal, adjacent dinuclear molecules are linked to the lattice water molecules, generating an $O-H \cdots O$ - and $N-H \cdots O$ -connected three-dimensional network. In the crystal, the hydroxy H atom is disordered over two positions in a 1:1 ratio; one half-occupancy H atom is connected to one hydroxy group, whereas the other half-occupancy H atom is connected to another hydroxy group.

Related literature

For the structure of 2-[(pyrimidin-2-yl)amino]methyl]phenol, see: Xu *et al.* (2011).



Experimental

Crystal data

$[Ag_2(C_{11}H_{10}N_3O)_2(C_{11}H_{11}N_3O)_2] \cdot 2H_2O$
 $M_r = 1054.67$
 Monoclinic, $P2_1/c$
 $a = 9.2992(4)$ Å
 $b = 24.808(1)$ Å
 $c = 9.8158(5)$ Å
 $\beta = 108.453(1)^\circ$
 $V = 2148.02(17)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.98$ mm⁻¹
 $T = 293$ K
 $0.23 \times 0.20 \times 0.17$ mm

Data collection

Rigaku R-Axis RAPID IP diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{min} = 0.807$, $T_{max} = 0.852$
 20943 measured reflections
 4910 independent reflections
 3230 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.133$
 $S = 1.11$
 4910 reflections
 307 parameters
 7 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 1.27$ e Å⁻³
 $\Delta\rho_{min} = -1.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1o \cdots O2^i$	0.84 (1)	1.68 (3)	2.504 (4)	166 (12)
$O2-H2o \cdots O1^{ii}$	0.84 (1)	1.68 (3)	2.504 (4)	166 (13)
$O1w-H11 \cdots O2^{iii}$	0.84 (1)	2.31 (6)	2.927 (5)	130 (6)
$O1w-H12 \cdots N3^{iv}$	0.84 (1)	2.27 (2)	3.085 (5)	165 (6)
$N1-H1 \cdots O1^v$	0.88 (1)	1.99 (1)	2.863 (5)	176 (4)
$N6-H6 \cdots O1w$	0.88 (1)	2.08 (2)	2.943 (5)	169 (5)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5644).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MS (2002). *CrystalClear*. Rigaku/MS Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Xu, J., Gao, S. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o3258.

supporting information

Acta Cryst. (2012). E68, m1538–m1539 [doi:10.1107/S1600536812045783]

**Bis{ μ -2-[(pyrimidin-2-yl)aminomethyl]phenolato}- κ^2 N¹:O; κ^2 O:N¹-bis-
(2-[(pyrimidin-2-yl- κ N)aminomethyl]phenol)silver(I)} dihydrate**

Shan Gao and Seik Weng Ng

S1. Comment

A recent study reports 2-[(pyrimidin-2-yl)aminomethyl]phenol, a reduced Schiff-base that possesses an acidic phenolic group (Xu *et al.*, 2011). The reaction with silver nitrate yields dinuclear $[\text{Ag}(\text{C}_{11}\text{H}_{10}\text{N}_3\text{O})(\text{C}_{11}\text{H}_{11}\text{N}_3\text{O})]_2 \cdot 2\text{H}_2\text{O}$ (Scheme I, Fig. 1). The asymmetric unit has one Ag atom; however, the hydroxy H-atom is disordered over two positions in a 1:1 ratio. One half-occupancy H-atom is connected to O1 whereas the other half-occupancy atom is connected to O2. The Ag^I atom shows *T*-shaped coordination. Adjacent molecules are linked to the lattice water molecules to generate a O–H \cdots O and N–H \cdots O connected three-dimensional network (Table 1).

S2. Experimental

An acetonitrile solution (10 ml) of silver nitrate (1 mmol) was added to a methanol solution (5 ml) of 2-[(pyrimidin-2-yl)aminomethyl]phenol (1 mmol) and potassium hydroxide (0.5 mmol). The solution was filtered and then side aside, away from light, for the growth of crystals. Colorless crystals were obtained after several days.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$. The amino and hydroxy/water H atoms were located in a difference Fourier map, and were refined with distance restraints of N–H 0.88±0.01, O–H 0.84±0.01 and H \cdots H 1.37±0.01 Å. Their temperature factors were refined.

The hydroxy H-atom is disordered over two positions in a 1:1 ratio; one half-occupancy H-atom is connected to O1 whereas the other half-occupancy atom is connected to O2.

The final difference Fourier map had a peak at 0.83 Å from Ag1 and a hole at 0.84 Å from this atom.

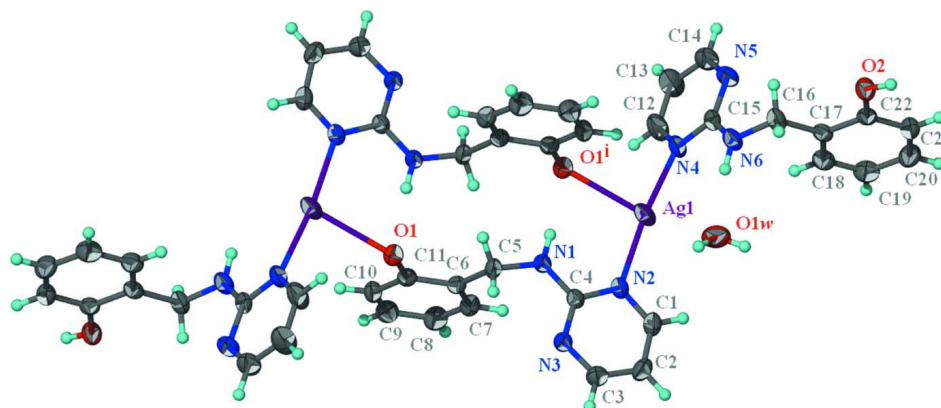


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[\text{Ag}_2(\text{C}_{11}\text{H}_{10}\text{N}_3\text{O})_2(\text{C}_{11}\text{H}_{11}\text{N}_3\text{O})_2]\cdot 2\text{H}_2\text{O}$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the phenolic –OH groups is not shown.

Bis[μ -2-[(pyrimidin-2-yl)aminomethyl]phenolato]- $\kappa^2\text{N}^1\text{O};\kappa^2\text{O}:\text{N}^1$ -bis[2-[(pyrimidin-2-yl)- κN]aminomethyl]phenol]silver(I) dihydrate

Crystal data

$[\text{Ag}_2(\text{C}_{11}\text{H}_{10}\text{N}_3\text{O})_2(\text{C}_{11}\text{H}_{11}\text{N}_3\text{O})_2]\cdot 2\text{H}_2\text{O}$

$M_r = 1054.67$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.2992$ (4) Å

$b = 24.808$ (1) Å

$c = 9.8158$ (5) Å

$\beta = 108.453$ (1)°

$V = 2148.02$ (17) Å³

$Z = 2$

$F(000) = 1072$

$D_x = 1.631$ Mg m⁻³

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

Cell parameters from 13157 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 0.98$ mm⁻¹

$T = 293$ K

Prism, colorless

$0.23 \times 0.20 \times 0.17$ mm

Data collection

Rigaku R-AXIS RAPID IP
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scan

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.807$, $T_{\max} = 0.852$

20943 measured reflections

4910 independent reflections

3230 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.1$ °

$h = -12 \rightarrow 11$

$k = -32 \rightarrow 32$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.133$

$S = 1.11$

4910 reflections

307 parameters

7 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

$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 4.7243P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.27$ e Å⁻³

$\Delta\rho_{\min} = -1.29$ e Å⁻³

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ag1	0.70167 (5)	0.644035 (13)	0.56817 (5)	0.04905 (15)	
O1	1.0721 (3)	0.39077 (12)	0.5102 (3)	0.0383 (7)	
H1O	0.990 (7)	0.376 (4)	0.461 (10)	0.057*	0.50
O2	0.1768 (4)	0.84419 (14)	0.0994 (4)	0.0458 (8)	
H2O	0.095 (7)	0.858 (5)	0.050 (11)	0.069*	0.50
O1W	0.3708 (5)	0.64557 (15)	0.4170 (5)	0.0650 (11)	
H11	0.289 (4)	0.659 (2)	0.420 (8)	0.097*	
H12	0.353 (6)	0.6145 (12)	0.382 (7)	0.097*	
N1	0.8011 (4)	0.51659 (14)	0.5833 (4)	0.0371 (9)	
H1	0.838 (5)	0.5460 (11)	0.557 (5)	0.045*	
N2	0.6393 (4)	0.56969 (14)	0.6588 (4)	0.0362 (8)	
N3	0.6313 (4)	0.47353 (14)	0.6741 (4)	0.0404 (9)	
N4	0.7537 (4)	0.72440 (15)	0.5013 (5)	0.0441 (10)	
N5	0.7062 (5)	0.80270 (15)	0.3525 (5)	0.0482 (10)	
N6	0.5199 (4)	0.73932 (15)	0.3360 (5)	0.0441 (10)	
H6	0.487 (6)	0.7108 (13)	0.370 (5)	0.053*	
C1	0.5302 (5)	0.57248 (19)	0.7213 (6)	0.0451 (11)	
H1A	0.4953	0.6062	0.7375	0.054*	
C2	0.4682 (5)	0.5276 (2)	0.7621 (6)	0.0472 (12)	
H2A	0.3940	0.5301	0.8069	0.057*	
C3	0.5215 (6)	0.4788 (2)	0.7332 (6)	0.0482 (12)	
H3	0.4785	0.4477	0.7562	0.058*	
C4	0.6884 (5)	0.51959 (16)	0.6398 (5)	0.0328 (9)	
C5	0.8671 (5)	0.46637 (17)	0.5550 (5)	0.0350 (9)	
H5A	0.8979	0.4710	0.4701	0.042*	
H5B	0.7897	0.4386	0.5339	0.042*	
C6	1.0024 (5)	0.44711 (17)	0.6770 (5)	0.0350 (9)	
C7	1.0368 (6)	0.4667 (2)	0.8155 (5)	0.0443 (11)	
H7	0.9729	0.4919	0.8365	0.053*	
C8	1.1647 (6)	0.4494 (2)	0.9240 (6)	0.0533 (13)	
H8	1.1873	0.4635	1.0162	0.064*	
C9	1.2577 (6)	0.4113 (2)	0.8933 (6)	0.0499 (12)	
H9	1.3435	0.3995	0.9653	0.060*	
C10	1.2245 (5)	0.39041 (18)	0.7566 (5)	0.0404 (10)	
H10	1.2873	0.3641	0.7384	0.048*	
C11	1.0981 (5)	0.40809 (16)	0.6445 (5)	0.0347 (9)	
C12	0.8956 (6)	0.7416 (2)	0.5634 (7)	0.0660 (17)	
H12A	0.9608	0.7209	0.6360	0.079*	
C13	0.9484 (7)	0.7889 (2)	0.5233 (9)	0.078 (2)	
H13	1.0475	0.8005	0.5669	0.094*	
C14	0.8486 (6)	0.8178 (2)	0.4167 (7)	0.0580 (14)	
H14	0.8819	0.8498	0.3875	0.070*	
C15	0.6627 (5)	0.75617 (17)	0.3970 (5)	0.0392 (10)	
C16	0.4023 (6)	0.77407 (18)	0.2440 (5)	0.0446 (11)	
H16A	0.3197	0.7516	0.1869	0.054*	

H16B	0.4437	0.7930	0.1783	0.054*
C17	0.3390 (5)	0.81517 (17)	0.3238 (5)	0.0355 (10)
C18	0.3894 (6)	0.82048 (19)	0.4713 (5)	0.0447 (11)
H18	0.4671	0.7983	0.5255	0.054*
C19	0.3273 (6)	0.8580 (2)	0.5401 (6)	0.0502 (12)
H19	0.3628	0.8609	0.6396	0.060*
C20	0.2126 (6)	0.8911 (2)	0.4609 (6)	0.0503 (12)
H20	0.1701	0.9163	0.5069	0.060*
C21	0.1606 (6)	0.88692 (19)	0.3134 (6)	0.0462 (12)
H21	0.0834	0.9095	0.2604	0.055*
C22	0.2225 (5)	0.84915 (17)	0.2430 (5)	0.0361 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0552 (3)	0.02896 (19)	0.0589 (3)	0.00169 (16)	0.01237 (19)	0.00829 (16)
O1	0.0365 (17)	0.0369 (16)	0.0407 (19)	-0.0016 (14)	0.0111 (15)	-0.0062 (13)
O2	0.047 (2)	0.0487 (19)	0.0391 (19)	0.0124 (16)	0.0096 (16)	0.0051 (15)
O1W	0.076 (3)	0.048 (2)	0.081 (3)	-0.020 (2)	0.040 (3)	-0.005 (2)
N1	0.036 (2)	0.0258 (17)	0.054 (2)	0.0002 (15)	0.0206 (19)	0.0032 (16)
N2	0.0352 (19)	0.0296 (17)	0.042 (2)	0.0038 (16)	0.0092 (17)	-0.0002 (15)
N3	0.040 (2)	0.0309 (18)	0.055 (3)	0.0011 (16)	0.0223 (19)	0.0027 (17)
N4	0.036 (2)	0.0319 (19)	0.061 (3)	0.0074 (17)	0.011 (2)	0.0106 (18)
N5	0.054 (3)	0.036 (2)	0.055 (3)	0.0006 (19)	0.018 (2)	0.0101 (18)
N6	0.042 (2)	0.0288 (19)	0.058 (3)	0.0006 (17)	0.010 (2)	0.0057 (18)
C1	0.043 (3)	0.040 (2)	0.053 (3)	0.009 (2)	0.018 (2)	-0.003 (2)
C2	0.035 (2)	0.060 (3)	0.050 (3)	0.006 (2)	0.019 (2)	0.000 (2)
C3	0.044 (3)	0.043 (3)	0.062 (3)	-0.002 (2)	0.023 (3)	0.007 (2)
C4	0.029 (2)	0.028 (2)	0.039 (2)	-0.0002 (17)	0.0069 (19)	0.0012 (17)
C5	0.030 (2)	0.031 (2)	0.046 (3)	0.0026 (18)	0.014 (2)	-0.0020 (18)
C6	0.035 (2)	0.032 (2)	0.040 (2)	-0.0017 (18)	0.016 (2)	0.0007 (18)
C7	0.047 (3)	0.045 (3)	0.044 (3)	0.007 (2)	0.020 (2)	0.000 (2)
C8	0.056 (3)	0.062 (3)	0.040 (3)	0.004 (3)	0.014 (3)	-0.001 (2)
C9	0.044 (3)	0.059 (3)	0.045 (3)	0.005 (2)	0.011 (2)	0.009 (2)
C10	0.035 (2)	0.038 (2)	0.048 (3)	0.007 (2)	0.012 (2)	0.003 (2)
C11	0.036 (2)	0.030 (2)	0.041 (3)	-0.0045 (18)	0.015 (2)	-0.0016 (18)
C12	0.042 (3)	0.052 (3)	0.095 (5)	0.010 (3)	0.008 (3)	0.022 (3)
C13	0.040 (3)	0.058 (4)	0.131 (6)	-0.005 (3)	0.017 (4)	0.022 (4)
C14	0.053 (3)	0.044 (3)	0.079 (4)	-0.004 (3)	0.024 (3)	0.010 (3)
C15	0.042 (3)	0.028 (2)	0.050 (3)	0.0072 (19)	0.019 (2)	0.0009 (19)
C16	0.044 (3)	0.033 (2)	0.053 (3)	0.005 (2)	0.010 (2)	0.002 (2)
C17	0.036 (2)	0.030 (2)	0.039 (2)	-0.0042 (18)	0.009 (2)	0.0043 (18)
C18	0.045 (3)	0.041 (2)	0.047 (3)	-0.004 (2)	0.013 (2)	0.004 (2)
C19	0.060 (3)	0.054 (3)	0.036 (3)	-0.007 (3)	0.013 (2)	-0.003 (2)
C20	0.055 (3)	0.051 (3)	0.051 (3)	0.002 (2)	0.025 (3)	-0.007 (2)
C21	0.045 (3)	0.040 (3)	0.057 (3)	0.007 (2)	0.021 (3)	0.004 (2)
C22	0.033 (2)	0.035 (2)	0.041 (2)	-0.0045 (18)	0.013 (2)	0.0049 (18)

Geometric parameters (Å, °)

Ag1—N4	2.200 (4)	C5—H5A	0.9700
Ag1—N2	2.204 (4)	C5—H5B	0.9700
Ag1—O1 ⁱ	2.606 (3)	C6—C7	1.382 (6)
Ag1—O1W	2.963 (5)	C6—C11	1.419 (6)
O1—C11	1.333 (5)	C7—C8	1.389 (7)
O1—H1O	0.840 (10)	C7—H7	0.9300
O2—C22	1.343 (5)	C8—C9	1.379 (7)
O2—H2O	0.839 (10)	C8—H8	0.9300
O1W—H11	0.842 (10)	C9—C10	1.379 (7)
O1W—H12	0.840 (10)	C9—H9	0.9300
N1—C4	1.334 (5)	C10—C11	1.402 (6)
N1—C5	1.454 (5)	C10—H10	0.9300
N1—H1	0.877 (10)	C12—C13	1.376 (8)
N2—C1	1.343 (6)	C12—H12A	0.9300
N2—C4	1.357 (5)	C13—C14	1.363 (8)
N3—C3	1.331 (6)	C13—H13	0.9300
N3—C4	1.347 (5)	C14—H14	0.9300
N4—C12	1.336 (7)	C16—C17	1.514 (6)
N4—C15	1.356 (6)	C16—H16A	0.9700
N5—C14	1.328 (7)	C16—H16B	0.9700
N5—C15	1.341 (6)	C17—C18	1.379 (6)
N6—C15	1.340 (6)	C17—C22	1.403 (6)
N6—C16	1.459 (6)	C18—C19	1.379 (7)
N6—H6	0.877 (10)	C18—H18	0.9300
C1—C2	1.371 (7)	C19—C20	1.375 (7)
C1—H1A	0.9300	C19—H19	0.9300
C2—C3	1.371 (7)	C20—C21	1.377 (7)
C2—H2A	0.9300	C20—H20	0.9300
C3—H3	0.9300	C21—C22	1.393 (6)
C5—C6	1.514 (6)	C21—H21	0.9300
N4—Ag1—N2	171.75 (14)	C9—C8—C7	119.2 (5)
N4—Ag1—O1 ⁱ	86.43 (12)	C9—C8—H8	120.4
N2—Ag1—O1 ⁱ	100.50 (11)	C7—C8—H8	120.4
N4—Ag1—O1W	97.51 (13)	C10—C9—C8	120.5 (5)
N2—Ag1—O1W	81.30 (12)	C10—C9—H9	119.7
O1 ⁱ —Ag1—O1W	131.60 (11)	C8—C9—H9	119.7
C11—O1—H1O	124 (8)	C9—C10—C11	121.4 (4)
C22—O2—H2O	120 (9)	C9—C10—H10	119.3
Ag1—O1W—H11	142 (4)	C11—C10—H10	119.3
Ag1—O1W—H12	103 (4)	O1—C11—C10	121.3 (4)
H11—O1W—H12	109 (2)	O1—C11—C6	120.8 (4)
C4—N1—C5	124.2 (3)	C10—C11—C6	117.8 (4)
C4—N1—H1	120 (3)	N4—C12—C13	122.1 (5)
C5—N1—H1	115 (3)	N4—C12—H12A	118.9
C1—N2—C4	116.5 (4)	C13—C12—H12A	118.9

C1—N2—Ag1	118.3 (3)	C14—C13—C12	116.8 (5)
C4—N2—Ag1	124.6 (3)	C14—C13—H13	121.6
C3—N3—C4	116.3 (4)	C12—C13—H13	121.6
C12—N4—C15	116.7 (4)	N5—C14—C13	123.3 (5)
C12—N4—Ag1	115.6 (3)	N5—C14—H14	118.3
C15—N4—Ag1	127.5 (3)	C13—C14—H14	118.3
C14—N5—C15	116.5 (4)	N6—C15—N5	118.8 (4)
C15—N6—C16	122.4 (4)	N6—C15—N4	116.8 (4)
C15—N6—H6	120 (4)	N5—C15—N4	124.5 (4)
C16—N6—H6	115 (4)	N6—C16—C17	114.6 (4)
N2—C1—C2	122.7 (4)	N6—C16—H16A	108.6
N2—C1—H1A	118.7	C17—C16—H16A	108.6
C2—C1—H1A	118.7	N6—C16—H16B	108.6
C3—C2—C1	116.3 (4)	C17—C16—H16B	108.6
C3—C2—H2A	121.8	H16A—C16—H16B	107.6
C1—C2—H2A	121.8	C18—C17—C22	118.8 (4)
N3—C3—C2	123.7 (4)	C18—C17—C16	123.3 (4)
N3—C3—H3	118.2	C22—C17—C16	118.0 (4)
C2—C3—H3	118.2	C19—C18—C17	121.5 (5)
N1—C4—N3	118.7 (4)	C19—C18—H18	119.3
N1—C4—N2	116.8 (4)	C17—C18—H18	119.3
N3—C4—N2	124.4 (4)	C20—C19—C18	119.7 (5)
N1—C5—C6	114.5 (4)	C20—C19—H19	120.1
N1—C5—H5A	108.6	C18—C19—H19	120.1
C6—C5—H5A	108.6	C19—C20—C21	120.1 (5)
N1—C5—H5B	108.6	C19—C20—H20	120.0
C6—C5—H5B	108.6	C21—C20—H20	120.0
H5A—C5—H5B	107.6	C20—C21—C22	120.6 (5)
C7—C6—C11	119.6 (4)	C20—C21—H21	119.7
C7—C6—C5	122.9 (4)	C22—C21—H21	119.7
C11—C6—C5	117.4 (4)	O2—C22—C21	122.6 (4)
C6—C7—C8	121.5 (4)	O2—C22—C17	118.0 (4)
C6—C7—H7	119.3	C21—C22—C17	119.3 (4)
C8—C7—H7	119.3		
O1 ⁱ —Ag1—N2—C1	175.4 (3)	C7—C6—C11—O1	-176.3 (4)
O1W—Ag1—N2—C1	-53.7 (3)	C5—C6—C11—O1	2.4 (6)
O1 ⁱ —Ag1—N2—C4	-13.9 (4)	C7—C6—C11—C10	0.7 (6)
O1W—Ag1—N2—C4	117.0 (4)	C5—C6—C11—C10	179.4 (4)
O1 ⁱ —Ag1—N4—C12	-55.8 (4)	C15—N4—C12—C13	-0.6 (9)
O1W—Ag1—N4—C12	172.7 (4)	Ag1—N4—C12—C13	174.3 (5)
O1 ⁱ —Ag1—N4—C15	118.4 (4)	N4—C12—C13—C14	0.2 (11)
O1W—Ag1—N4—C15	-13.1 (4)	C15—N5—C14—C13	-0.4 (9)
C4—N2—C1—C2	-1.1 (7)	C12—C13—C14—N5	0.4 (10)
Ag1—N2—C1—C2	170.3 (4)	C16—N6—C15—N5	-12.2 (7)
N2—C1—C2—C3	-1.2 (8)	C16—N6—C15—N4	167.5 (4)
C4—N3—C3—C2	-1.3 (8)	C14—N5—C15—N6	179.7 (5)
C1—C2—C3—N3	2.6 (8)	C14—N5—C15—N4	-0.1 (7)

C5—N1—C4—N3	0.4 (7)	C12—N4—C15—N6	-179.2 (5)
C5—N1—C4—N2	-179.7 (4)	Ag1—N4—C15—N6	6.6 (6)
C3—N3—C4—N1	178.5 (4)	C12—N4—C15—N5	0.6 (7)
C3—N3—C4—N2	-1.4 (7)	Ag1—N4—C15—N5	-173.6 (3)
C1—N2—C4—N1	-177.3 (4)	C15—N6—C16—C17	-77.1 (6)
Ag1—N2—C4—N1	11.8 (6)	N6—C16—C17—C18	1.2 (6)
C1—N2—C4—N3	2.6 (7)	N6—C16—C17—C22	-178.3 (4)
Ag1—N2—C4—N3	-168.3 (3)	C22—C17—C18—C19	0.5 (7)
C4—N1—C5—C6	-91.6 (5)	C16—C17—C18—C19	-179.1 (4)
N1—C5—C6—C7	16.3 (6)	C17—C18—C19—C20	-0.1 (7)
N1—C5—C6—C11	-162.4 (4)	C18—C19—C20—C21	-0.3 (8)
C11—C6—C7—C8	0.8 (7)	C19—C20—C21—C22	0.4 (7)
C5—C6—C7—C8	-177.8 (4)	C20—C21—C22—O2	-179.1 (4)
C6—C7—C8—C9	-1.2 (8)	C20—C21—C22—C17	0.0 (7)
C7—C8—C9—C10	0.1 (8)	C18—C17—C22—O2	178.7 (4)
C8—C9—C10—C11	1.5 (7)	C16—C17—C22—O2	-1.7 (6)
C9—C10—C11—O1	175.2 (4)	C18—C17—C22—C21	-0.4 (6)
C9—C10—C11—C6	-1.9 (6)	C16—C17—C22—C21	179.2 (4)

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

Hydrogen-bond geometry (Å, °)

<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>
O1—H1o...O2 ⁱⁱ	0.84 (1)	1.68 (3)	2.504 (4)	166 (12)
O2—H2o...O1 ⁱⁱⁱ	0.84 (1)	1.68 (3)	2.504 (4)	166 (13)
O1w—H11...O2 ^{iv}	0.84 (1)	2.31 (6)	2.927 (5)	130 (6)
O1w—H12...N3 ^v	0.84 (1)	2.27 (2)	3.085 (5)	165 (6)
N1—H1...O1 ⁱ	0.88 (1)	1.99 (1)	2.863 (5)	176 (4)
N6—H6...O1w	0.88 (1)	2.08 (2)	2.943 (5)	169 (5)

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