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Bis(2,5-di-4-pyridyl-1,3,4-oxadiazole)-silver(I) nitrate monohydrate

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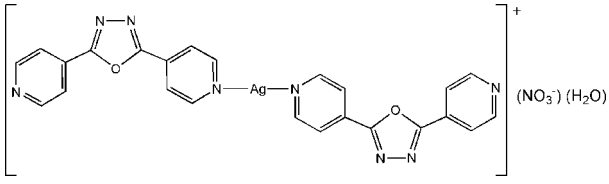
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.085; data-to-parameter ratio = 11.9.

In the title mononuclear complex, $[Ag(C_{12}H_8N_4O)_2]NO_3\cdot H_2O$, the Ag^I ion is coordinated linearly by two pyridyl N atoms from two crystallographically independent monodentate 2,5-di-4-pyridyl-1,3,4-oxadiazole (4-bpo) ligands. In addition, the asymmetric unit contains one nitrate anion and one solvent water molecule. In the crystal structure, nitrate anions connect to Ag^I ions *via* weak Ag···O interactions [Ag···O = 2.836 (3) Å] and to two symmetry-related solvent water molecules *via* O—H···O hydrogen bonds, to afford a one-dimensional herring-bone-like motif along [100]. Significant π–π stacking interactions [$Cg\cdots Cg$ = 3.614 (2)–3.721 (2) Å, where Cg is the centroid of a pyridyl or oxadiazole ring] are also found between two adjacent one-dimensional motifs, resulting in a double-strand supramolecular array.

Related literature

For related literature, see: Dong *et al.* (2003); Du & Zhao (2004); Du *et al.* (2005, 2006, 2007); Guo *et al.* (2003).



Experimental

Crystal data

$[Ag(C_{12}H_8N_4O)_2]NO_3\cdot H_2O$
M_r = 636.34
Monoclinic, $P2_1/n$
a = 7.3200 (19) Å
b = 13.281 (3) Å
c = 25.002 (6) Å
β = 92.664 (3)°
V = 2428.0 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 294 (2) K
0.14 × 0.13 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.781, T_{max} = 0.849
(expected range = 0.849–0.923)
13051 measured reflections
4287 independent reflections
3232 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.02
4287 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.171 (2)	Ag1—N5	2.173 (2)
N1—Ag1—N5	179.10 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O4^{i}	0.85	2.22	2.949 (5)	144
O6—H6B···O3	0.85	2.29	3.014 (5)	144
C4—H4···O5^{ii}	0.93	2.49	3.228 (4)	137
C5—H5···N2^{iii}	0.93	2.55	3.443 (3)	161
C9—H9···O4^{iv}	0.93	2.58	3.197 (4)	125
C15—H15···O3^{ii}	0.93	2.56	3.481 (4)	169
C17—H17···N6^{v}	0.93	2.57	3.467 (3)	163

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2* and *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and *DIAMOND* (Brandenburg, 2005); 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: LH2554).

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supplementary materials

Acta Cryst. (2007). E**63**, m3044 [**doi:10.1107/S1600536807057546**]

Bis(2,5-di-4-pyridyl-1,3,4-oxadiazole)silver(I) nitrate monohydrate

Z.-H. Zhang, C.-P. Li, Y.-L. Tian and Y.-M. Guo

Comment

The angular dipyridyl ligand, 2,5-di-4-pyridyl-1,3,4-oxadiazole (4-bpo), has been demonstrated to be an excellent building block to assemble with familiar transition metal ions, which produces a variety of coordination complexes from 0-D to 3-D (Du *et al.*, 2005, 2006, 2007). With respect to Ag^{I} complexes, these are usually coordination polymers with infinite coordination arrays, in which the 4-bpo ligands display either μ-N_{py}, N_{py} or μ_3-N_{py}, N_{py}, $N_{oxadiazole}$ bridging coordination modes (Dong *et al.*, 2003; Du & Zhao, 2004). For instance, self-assembly of $AgNO_3$ with 4-bpo through slow diffusion in $CH_3CN/CHCl_3$ yields a chain complex [Ag(4-bpo)(NO_3)], in which the trigonal Ag^{I} centers are bridged by 4-bpo in μ-N_{py}, N_{py} fashion (Guo *et al.*, 2003). Herein, we describe a related complex [Ag(4-bpo)$_2$](NO_3)(H_2O) (I) prepared under hydrothermal condition, which has an unexpected mononuclear structure.

The molecular structure of the title compound (I) is shown in Fig. 1. The Ag^{I} ion is coordinated by two N atoms of the pyridyl rings from two separate monodentate 4-bpo ligands in *trans*-arrangement [Ag1—N1 = 2.171 (2) Å and Ag1—N5 = 2.173 (2) Å], displaying a linear geometry [N1—Ag1—N5 = 179.10 (8)°]. There is also a weak Ag1—O5 (2.836 (3) Å) contact between each Ag^{I} center and the adjacent nitrate anion. The two pyridyl rings in one 4-bpo ligand are inclined by 7.9 (4) and 12.7 (4)° with respect to the central oxadiazole plane, and by 10.6 (1)° with respect to each other. Corresponding values for the other 4-bpo molecule are 5.9 (2), 13.3 (1), and 10.7 (2)°. Interestingly, each nitrate acts as the acceptor of a pair of O—H···O bonds with the neighboring two water molecules, and thus, a supramolecular chain along the [100] direction is afforded. Two adjacent such 1-D chains are interdigitated and further combined to give a double-strand supramolecular array (see Fig. 2), *via* interchain parallel π–π stacking forces (center-to-center distances between the corresponding aromatic rings in 4-bpo are in the range of 3.61–3.72 Å). In addition, multiple C—H···O and C—H···N interactions (see Table) are observed to consolidate this crystalline lattice.

Experimental

A water (8 ml) solution containing $AgNO_3$ (17.3 mg, 0.1 mmol), 4-bpo (11.2 mg, 0.05 mmol), and oxamide (9.0 mg, 0.1 mmol) was sealed in a Teflon-lined stainless steel vessel (20 ml), which was heated to 373 K for 24 h and subsequently cooled to room temperature at a rate of 1 K/h. Colorless block shape crystals were obtained in 75% yield (11.9 mg, based on 4-bpo). IR (cm^{-1}): 3385*b*, 2362*s*, 1654*s*, 1563*m*, 1536*m*, 1484*m*, 1416*m*, 1384*vs*, 1106*m*, 988*w*, 832*m*, 741*w*, 713*s*, 637*w*.

Refinement

C-bound hydrogen atoms were placed geometrically C—H = 0.93 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). Hydrogen atoms bonded to the water O atom were visible in difference Fourier maps, but were fixed geometrically with O—H = 0.85 Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

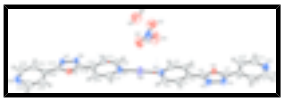

Fig. 1. Molecular structure of with atom labeling of all non-H atoms, shown with 30% probability displacement ellipsoids.

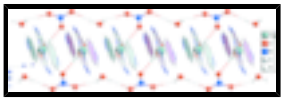

Fig. 2. One-dimensional double-strand supramolecular array of (I) extending along the [100] direction. H atoms of 4-bpo are omitted for clarity. Hydrogen bonds are shown with dashed lines.

s(2,5-di-4-pyridyl-1,3,4-oxadiazole)silver(I) nitrate monohydrate

Crystal data

$[Ag(C_{12}H_8N_4O)_2]NO_3·H_2O$	F_{000} = 1280
M_r = 636.34	D_x = 1.741 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4561 reflections
a = 7.3200 (19) Å	θ = 2.2–25.8º
b = 13.281 (3) Å	μ = 0.89 mm^{-1}
c = 25.002 (6) Å	T = 294 (2) K
β = 92.664 (3)º	Block, colourless
V = 2428.0 (11) Å^3	0.14 × 0.13 × 0.09 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	4287 independent reflections
Radiation source: fine-focus sealed tube	3232 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −8→7
T_{min} = 0.781, T_{max} = 0.849	k = −15→15
13051 measured reflections	l = −29→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H-atom parameters constrained
$wR(F^2)$ = 0.085	$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 1.1166P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001

4287 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.75772 (4)	0.494095 (15)	0.003989 (9)	0.06022 (12)
O1	0.7828 (2)	0.01648 (12)	0.14056 (6)	0.0331 (4)
O2	0.7228 (2)	0.96348 (13)	−0.13712 (6)	0.0353 (4)
O3	0.3960 (5)	0.5442 (2)	0.15393 (12)	0.0977 (9)
O4	0.6848 (4)	0.5320 (2)	0.14858 (12)	0.0962 (9)
O5	0.5187 (5)	0.5726 (2)	0.07974 (11)	0.1103 (11)
N1	0.7338 (3)	0.34138 (15)	0.03382 (8)	0.0400 (5)
N2	0.6208 (3)	−0.03195 (16)	0.06841 (8)	0.0390 (5)
N3	0.6508 (3)	−0.11581 (15)	0.10182 (8)	0.0394 (5)
N4	0.9379 (4)	−0.26272 (19)	0.27527 (9)	0.0542 (6)
N5	0.7790 (3)	0.64634 (16)	−0.02698 (9)	0.0422 (5)
N6	0.8743 (3)	1.02181 (15)	−0.06527 (8)	0.0385 (5)
N7	0.8432 (3)	1.10181 (16)	−0.10126 (8)	0.0403 (5)
N8	0.5575 (4)	1.2125 (2)	−0.28380 (10)	0.0635 (8)
N9	0.5326 (5)	0.55187 (18)	0.12635 (12)	0.0624 (8)
C1	0.7127 (3)	0.14629 (17)	0.07331 (9)	0.0294 (5)
C2	0.7864 (3)	0.22346 (18)	0.10502 (9)	0.0351 (6)
H2	0.8297	0.2108	0.1399	0.042*
C3	0.7942 (4)	0.31880 (19)	0.08386 (10)	0.0402 (6)
H3	0.8437	0.3701	0.1053	0.048*
C4	0.6629 (4)	0.26646 (19)	0.00361 (10)	0.0391 (6)
H4	0.6216	0.2810	−0.0313	0.047*
C5	0.6482 (4)	0.16930 (18)	0.02156 (9)	0.0354 (6)
H5	0.5960	0.1197	−0.0005	0.042*
C6	0.7006 (3)	0.04297 (18)	0.09256 (9)	0.0315 (6)
C7	0.7458 (3)	−0.08427 (18)	0.14297 (10)	0.0331 (6)
C8	0.8143 (4)	−0.14296 (19)	0.18910 (10)	0.0359 (6)
C9	0.8063 (4)	−0.2469 (2)	0.18619 (11)	0.0457 (7)

H9	0.7597	−0.2788	0.1554	0.055*
C10	0.8688 (4)	−0.3024 (2)	0.22991 (12)	0.0535 (8)
H10	0.8621	−0.3722	0.2275	0.064*
C11	0.9429 (4)	−0.1626 (2)	0.27713 (11)	0.0508 (8)
H11	0.9894	−0.1329	0.3086	0.061*
C12	0.8842 (4)	−0.0996 (2)	0.23588 (10)	0.0426 (7)
H12	0.8917	−0.0300	0.2395	0.051*
C13	0.7920 (3)	0.84052 (18)	−0.06722 (9)	0.0319 (6)
C14	0.7207 (4)	0.76235 (19)	−0.09872 (10)	0.0378 (6)
H14	0.6758	0.7742	−0.1336	0.045*
C15	0.7181 (4)	0.66720 (19)	−0.07716 (11)	0.0430 (7)
H15	0.6719	0.6148	−0.0984	0.052*
C16	0.8458 (4)	0.72245 (19)	0.00307 (10)	0.0399 (6)
H16	0.8871	0.7089	0.0381	0.048*
C17	0.8562 (4)	0.81970 (18)	−0.01540 (9)	0.0363 (6)
H17	0.9053	0.8705	0.0065	0.044*
C18	0.8010 (3)	0.94280 (18)	−0.08788 (9)	0.0324 (6)
C19	0.7541 (4)	1.06397 (18)	−0.14211 (10)	0.0348 (6)
C20	0.6850 (4)	1.1144 (2)	−0.19096 (10)	0.0379 (6)
C21	0.6799 (4)	1.2186 (2)	−0.19361 (11)	0.0467 (7)
H21	0.7187	1.2576	−0.1643	0.056*
C22	0.6162 (5)	1.2629 (3)	−0.24038 (13)	0.0594 (8)
H22	0.6138	1.3328	−0.2418	0.071*
C23	0.5636 (5)	1.1129 (3)	−0.28027 (12)	0.0640 (9)
H23	0.5237	1.0761	−0.3102	0.077*
C24	0.6249 (4)	1.0599 (2)	−0.23536 (11)	0.0510 (7)
H24	0.6255	0.9899	−0.2351	0.061*
O6	0.0299 (5)	0.5615 (2)	0.09432 (11)	0.1088 (10)
H6A	−0.0340	0.5408	0.1197	0.163*
H6B	0.1381	0.5810	0.1026	0.163*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0852 (2)	0.03234 (14)	0.06241 (18)	−0.00484 (12)	−0.00465 (14)	0.01112 (10)
O1	0.0375 (10)	0.0287 (9)	0.0324 (9)	−0.0012 (7)	−0.0035 (7)	0.0006 (7)
O2	0.0401 (11)	0.0334 (9)	0.0318 (9)	−0.0022 (8)	−0.0060 (8)	−0.0008 (7)
O3	0.118 (3)	0.0802 (19)	0.096 (2)	0.0038 (18)	0.0234 (19)	−0.0079 (16)
O4	0.106 (2)	0.0663 (16)	0.112 (2)	−0.0123 (16)	−0.0351 (19)	0.0043 (15)
O5	0.159 (3)	0.108 (2)	0.0636 (18)	0.023 (2)	−0.0036 (18)	0.0261 (16)
N1	0.0477 (15)	0.0320 (11)	0.0396 (12)	−0.0005 (10)	−0.0035 (10)	0.0025 (9)
N2	0.0454 (14)	0.0339 (11)	0.0370 (12)	−0.0049 (10)	−0.0072 (10)	0.0031 (9)
N3	0.0457 (15)	0.0327 (11)	0.0392 (12)	−0.0059 (10)	−0.0039 (10)	0.0039 (9)
N4	0.0566 (17)	0.0581 (16)	0.0474 (14)	0.0071 (13)	−0.0035 (12)	0.0134 (12)
N5	0.0515 (15)	0.0339 (11)	0.0409 (13)	−0.0007 (11)	−0.0010 (11)	0.0034 (9)
N6	0.0443 (14)	0.0330 (11)	0.0372 (12)	−0.0028 (10)	−0.0074 (10)	0.0013 (9)
N7	0.0482 (15)	0.0330 (11)	0.0389 (12)	−0.0030 (10)	−0.0073 (11)	0.0021 (9)
N8	0.0556 (18)	0.086 (2)	0.0479 (16)	0.0098 (15)	−0.0030 (13)	0.0239 (14)

N9	0.088 (2)	0.0349 (14)	0.0635 (19)	−0.0041 (15)	−0.0099 (18)	−0.0045 (12)
C1	0.0263 (14)	0.0315 (12)	0.0305 (13)	0.0004 (10)	0.0014 (10)	−0.0017 (9)
C2	0.0388 (16)	0.0366 (13)	0.0294 (12)	0.0001 (12)	−0.0038 (11)	−0.0026 (10)
C3	0.0475 (18)	0.0313 (13)	0.0413 (15)	−0.0042 (12)	−0.0023 (12)	−0.0060 (11)
C4	0.0459 (17)	0.0374 (14)	0.0335 (13)	0.0001 (13)	−0.0045 (12)	0.0025 (11)
C5	0.0389 (16)	0.0347 (13)	0.0320 (13)	−0.0014 (11)	−0.0035 (11)	−0.0040 (10)
C6	0.0307 (15)	0.0353 (13)	0.0282 (12)	−0.0004 (11)	−0.0001 (10)	−0.0012 (10)
C7	0.0340 (15)	0.0300 (13)	0.0354 (13)	−0.0021 (11)	0.0032 (11)	−0.0004 (10)
C8	0.0343 (15)	0.0387 (14)	0.0347 (13)	0.0006 (12)	0.0013 (11)	0.0054 (11)
C9	0.0520 (19)	0.0383 (14)	0.0459 (16)	−0.0030 (13)	−0.0073 (13)	0.0036 (12)
C10	0.059 (2)	0.0407 (15)	0.0601 (19)	0.0021 (15)	−0.0047 (16)	0.0110 (14)
C11	0.055 (2)	0.062 (2)	0.0354 (15)	0.0054 (16)	−0.0038 (13)	0.0010 (13)
C12	0.0473 (18)	0.0419 (15)	0.0384 (15)	0.0025 (13)	−0.0013 (13)	0.0002 (11)
C13	0.0296 (15)	0.0342 (13)	0.0319 (13)	0.0024 (11)	0.0006 (11)	−0.0002 (10)
C14	0.0420 (17)	0.0382 (14)	0.0325 (13)	−0.0034 (12)	−0.0051 (12)	−0.0018 (10)
C15	0.0513 (18)	0.0340 (14)	0.0431 (15)	−0.0065 (13)	−0.0042 (13)	−0.0060 (11)
C16	0.0469 (18)	0.0400 (14)	0.0323 (13)	0.0025 (13)	−0.0034 (12)	0.0033 (11)
C17	0.0397 (16)	0.0359 (13)	0.0331 (13)	−0.0021 (12)	−0.0019 (11)	−0.0051 (10)
C18	0.0298 (15)	0.0357 (14)	0.0315 (13)	0.0000 (11)	−0.0016 (11)	−0.0033 (10)
C19	0.0357 (16)	0.0336 (13)	0.0350 (14)	−0.0002 (11)	0.0013 (12)	0.0023 (10)
C20	0.0318 (15)	0.0475 (15)	0.0341 (14)	0.0018 (12)	0.0004 (11)	0.0041 (11)
C21	0.0520 (19)	0.0447 (16)	0.0436 (15)	0.0025 (14)	0.0017 (13)	0.0073 (12)
C22	0.057 (2)	0.063 (2)	0.058 (2)	0.0065 (17)	0.0033 (16)	0.0220 (16)
C23	0.060 (2)	0.093 (3)	0.0373 (17)	0.0018 (19)	−0.0141 (15)	0.0005 (16)
C24	0.054 (2)	0.0558 (18)	0.0427 (16)	0.0007 (15)	−0.0102 (14)	−0.0016 (13)
O6	0.129 (3)	0.121 (3)	0.0761 (19)	0.025 (2)	−0.0020 (18)	−0.0038 (17)

Geometric parameters (Å, °)

Ag1—N1	2.171 (2)	C5—H5	0.9300
Ag1—N5	2.173 (2)	C7—C8	1.461 (3)
O1—C6	1.364 (3)	C8—C12	1.381 (4)
O1—C7	1.367 (3)	C8—C9	1.384 (4)
O2—C19	1.361 (3)	C9—C10	1.378 (4)
O2—C18	1.361 (3)	C9—H9	0.9300
O3—N9	1.245 (4)	C10—H10	0.9300
O4—N9	1.250 (4)	C11—C12	1.381 (4)
O5—N9	1.197 (3)	C11—H11	0.9300
N1—C4	1.339 (3)	C12—H12	0.9300
N1—C3	1.341 (3)	C13—C17	1.385 (3)
N2—C6	1.289 (3)	C13—C14	1.390 (3)
N2—N3	1.403 (3)	C13—C18	1.456 (3)
N3—C7	1.285 (3)	C14—C15	1.374 (4)
N4—C10	1.329 (4)	C14—H14	0.9300
N4—C11	1.331 (4)	C15—H15	0.9300
N5—C16	1.338 (3)	C16—C17	1.375 (3)
N5—C15	1.341 (3)	C16—H16	0.9300
N6—C18	1.296 (3)	C17—H17	0.9300
N6—N7	1.404 (3)	C19—C20	1.462 (3)

N7—C19	1.288 (3)	C20—C24	1.380 (4)
N8—C23	1.327 (4)	C20—C21	1.386 (4)
N8—C22	1.329 (4)	C21—C22	1.371 (4)
C1—C2	1.389 (3)	C21—H21	0.9300
C1—C5	1.391 (3)	C22—H22	0.9300
C1—C6	1.458 (3)	C23—C24	1.383 (4)
C2—C3	1.375 (3)	C23—H23	0.9300
C2—H2	0.9300	C24—H24	0.9300
C3—H3	0.9300	O6—H6A	0.8505
C4—C5	1.372 (3)	O6—H6B	0.8501
C4—H4	0.9300		
N1—Ag1—N5	179.10 (8)	N4—C10—H10	117.8
C6—O1—C7	102.18 (18)	C9—C10—H10	117.8
C19—O2—C18	102.44 (18)	N4—C11—C12	124.9 (3)
C4—N1—C3	117.5 (2)	N4—C11—H11	117.5
C4—N1—Ag1	122.40 (17)	C12—C11—H11	117.5
C3—N1—Ag1	120.05 (17)	C8—C12—C11	118.0 (3)
C6—N2—N3	106.20 (19)	C8—C12—H12	121.0
C7—N3—N2	106.4 (2)	C11—C12—H12	121.0
C10—N4—C11	115.8 (2)	C17—C13—C14	118.9 (2)
C16—N5—C15	117.8 (2)	C17—C13—C18	119.9 (2)
C16—N5—Ag1	122.21 (17)	C14—C13—C18	121.2 (2)
C15—N5—Ag1	119.95 (17)	C15—C14—C13	118.4 (2)
C18—N6—N7	106.34 (19)	C15—C14—H14	120.8
C19—N7—N6	105.9 (2)	C13—C14—H14	120.8
C23—N8—C22	116.0 (3)	N5—C15—C14	123.2 (2)
O5—N9—O3	121.6 (4)	N5—C15—H15	118.4
O5—N9—O4	121.0 (4)	C14—C15—H15	118.4
O3—N9—O4	117.3 (3)	N5—C16—C17	123.0 (2)
C2—C1—C5	118.3 (2)	N5—C16—H16	118.5
C2—C1—C6	122.3 (2)	C17—C16—H16	118.5
C5—C1—C6	119.4 (2)	C16—C17—C13	118.7 (2)
C3—C2—C1	118.8 (2)	C16—C17—H17	120.7
C3—C2—H2	120.6	C13—C17—H17	120.7
C1—C2—H2	120.6	N6—C18—O2	112.3 (2)
N1—C3—C2	123.2 (2)	N6—C18—C13	128.7 (2)
N1—C3—H3	118.4	O2—C18—C13	119.0 (2)
C2—C3—H3	118.4	N7—C19—O2	113.0 (2)
N1—C4—C5	123.3 (2)	N7—C19—C20	128.8 (2)
N1—C4—H4	118.4	O2—C19—C20	118.2 (2)
C5—C4—H4	118.4	C24—C20—C21	118.6 (3)
C4—C5—C1	118.9 (2)	C24—C20—C19	121.1 (2)
C4—C5—H5	120.6	C21—C20—C19	120.3 (2)
C1—C5—H5	120.6	C22—C21—C20	118.4 (3)
N2—C6—O1	112.6 (2)	C22—C21—H21	120.8
N2—C6—C1	127.2 (2)	C20—C21—H21	120.8
O1—C6—C1	120.1 (2)	N8—C22—C21	124.4 (3)
N3—C7—O1	112.6 (2)	N8—C22—H22	117.8
N3—C7—C8	127.7 (2)	C21—C22—H22	117.8

O1—C7—C8	119.7 (2)	N8—C23—C24	124.8 (3)
C12—C8—C9	118.3 (2)	N8—C23—H23	117.6
C12—C8—C7	123.1 (2)	C24—C23—H23	117.6
C9—C8—C7	118.6 (2)	C20—C24—C23	117.7 (3)
C10—C9—C8	118.7 (3)	C20—C24—H24	121.1
C10—C9—H9	120.7	C23—C24—H24	121.1
C8—C9—H9	120.7	H6A—O6—H6B	117.1
N4—C10—C9	124.4 (3)		
C6—N2—N3—C7	−0.1 (3)	N4—C11—C12—C8	0.3 (5)
C18—N6—N7—C19	0.1 (3)	C17—C13—C14—C15	−0.5 (4)
C5—C1—C2—C3	−0.6 (4)	C18—C13—C14—C15	179.2 (2)
C6—C1—C2—C3	179.6 (2)	C16—N5—C15—C14	−0.2 (4)
C4—N1—C3—C2	0.0 (4)	Ag1—N5—C15—C14	177.4 (2)
Ag1—N1—C3—C2	−178.8 (2)	C13—C14—C15—N5	0.8 (4)
C1—C2—C3—N1	0.0 (4)	C15—N5—C16—C17	−0.7 (4)
C3—N1—C4—C5	0.6 (4)	Ag1—N5—C16—C17	−178.3 (2)
Ag1—N1—C4—C5	179.4 (2)	N5—C16—C17—C13	1.0 (4)
N1—C4—C5—C1	−1.2 (4)	C14—C13—C17—C16	−0.4 (4)
C2—C1—C5—C4	1.2 (4)	C18—C13—C17—C16	179.9 (2)
C6—C1—C5—C4	−179.0 (2)	N7—N6—C18—O2	0.4 (3)
N3—N2—C6—O1	−0.3 (3)	N7—N6—C18—C13	−178.9 (2)
N3—N2—C6—C1	178.2 (2)	C19—O2—C18—N6	−0.7 (3)
C7—O1—C6—N2	0.6 (3)	C19—O2—C18—C13	178.7 (2)
C7—O1—C6—C1	−178.1 (2)	C17—C13—C18—N6	5.0 (4)
C2—C1—C6—N2	173.4 (3)	C14—C13—C18—N6	−174.7 (3)
C5—C1—C6—N2	−6.4 (4)	C17—C13—C18—O2	−174.3 (2)
C2—C1—C6—O1	−8.2 (4)	C14—C13—C18—O2	6.1 (4)
C5—C1—C6—O1	172.0 (2)	N6—N7—C19—O2	−0.5 (3)
N2—N3—C7—O1	0.5 (3)	N6—N7—C19—C20	179.2 (3)
N2—N3—C7—C8	−179.2 (2)	C18—O2—C19—N7	0.7 (3)
C6—O1—C7—N3	−0.6 (3)	C18—O2—C19—C20	−179.0 (2)
C6—O1—C7—C8	179.1 (2)	N7—C19—C20—C24	166.7 (3)
N3—C7—C8—C12	−167.0 (3)	O2—C19—C20—C24	−13.6 (4)
O1—C7—C8—C12	13.3 (4)	N7—C19—C20—C21	−12.8 (4)
N3—C7—C8—C9	12.0 (4)	O2—C19—C20—C21	166.9 (2)
O1—C7—C8—C9	−167.7 (2)	C24—C20—C21—C22	−0.4 (4)
C12—C8—C9—C10	−0.2 (4)	C19—C20—C21—C22	179.2 (3)
C7—C8—C9—C10	−179.2 (3)	C23—N8—C22—C21	−0.3 (5)
C11—N4—C10—C9	0.7 (5)	C20—C21—C22—N8	0.3 (5)
C8—C9—C10—N4	−0.3 (5)	C22—N8—C23—C24	0.3 (5)
C10—N4—C11—C12	−0.7 (5)	C21—C20—C24—C23	0.4 (4)
C9—C8—C12—C11	0.2 (4)	C19—C20—C24—C23	−179.2 (3)
C7—C8—C12—C11	179.2 (3)	N8—C23—C24—C20	−0.3 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O4^{i}	0.85	2.22	2.949 (5)	144
O6—H6B···O3	0.85	2.29	3.014 (5)	144

C4—H4···O5^{ii}	0.93	2.49	3.228 (4)	137
C5—H5···N2^{iii}	0.93	2.55	3.443 (3)	161
C9—H9···O4^{iv}	0.93	2.58	3.197 (4)	125
C15—H15···O3^{ii}	0.93	2.56	3.481 (4)	169
C17—H17···N6^{v}	0.93	2.57	3.467 (3)	163

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*, −*z*; (iv) *x*, *y*−1, *z*; (v) −*x*+2, −*y*+2, −*z*.

Fig. 1

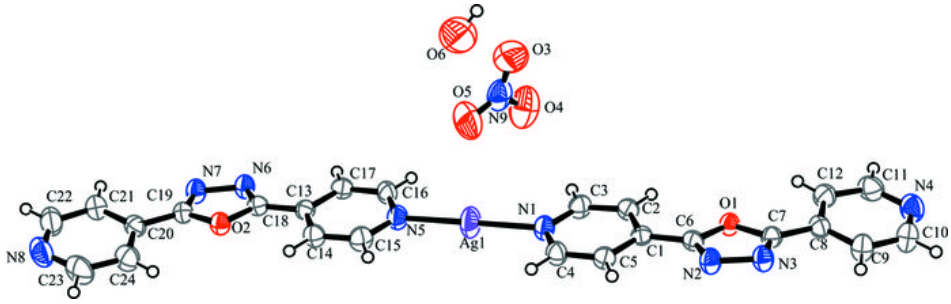
O6
O3
O5
N9
O4
N7
N6
C22
C21
C19
C13
C17
C12
C11
N4
C18
C16
C3
C2
O1
C6
C7
N8
C20
O2
C14
C15
N5
Ag1
N1
C1
C8
C10
C23
C24
C4
C5
N2
N3
C9

Fig. 2