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Synthesis, crystal structure and Hirshfeld surface analysis of a coordination compound of silver nitrate with 2-aminobenzoxazole

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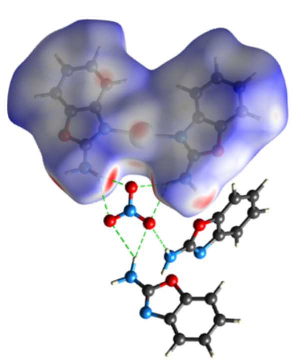
The coordination complex of 2-aminobenzaxole (2AB) with silver(I), namely, bis(2-aminobenzoxazole-κ*N*)silver(I) nitrate–bis(2-aminobenzoxazole (1/2), $[Ag(C_7H_6N_2O)_2]NO_3{\cdot}2C_7H_6N_2O$ or $[Ag(2AB)_2]NO_3{\cdot}(2AB)_2$, was synthesized from ethanol solutions of $AgNO_3$ and 2AB. The asymmetric unit contains one molecule of $[Ag(2AB)_2]NO_3{\cdot}(2AB)_2$, The central silver(I) atom is coordinated by two nitrogen donor atoms from 2-aminobenzaxazole ligands in an N_2 coordination set while another two 2-aminobenzaxazole ligands and one nitrate anion remain uncoordinated. The crystal structure features several intramolecular N—H···O and N—H···N hydrogen-bonding interactions as well as C—H···π, Ag···π and π–π interactions between adjacent AB ligands. Hirshfeld surface analysis and two-dimensional fingerprint plots were used to investigate the intermolecular interactions.



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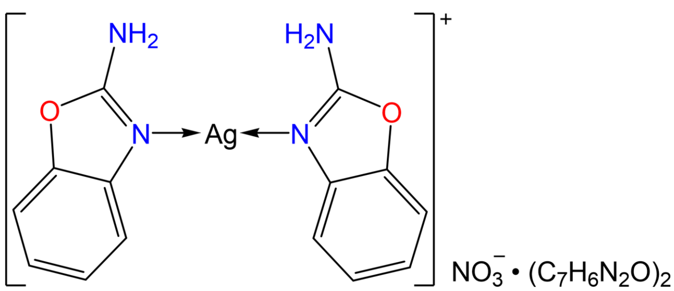
1. Chemical context

The benzoxazole framework has been explored for its antitubercular potential since the early 19th century (Wagner & Vonderbank, 1949; Šlachtová & Brulíková, 2018). In recent decades, 2-aminobenzoxazole (2AB) has attracted considerable attention due to its structural versatility and broad spectrum of applications in pharmaceuticals because of its antibacterial (Paramashivappa *et al.*, 2003), anti-inflammatory (Parlapalli & Manda, 2017), antitumour (Imaizumi *et al.*, 2020), antimicrobial (Erol *et al.*, 2022;), analgesic (Ali *et al.*, 2022; Sattar *et al.*, 2020) and fungicidal activities (Fan *et al.*, 2022), as well as in agrochemicals and materials science (Potashman *et al.*, 2007). Substituents at the 2- and 5-positions of the benzene ring have been found to significantly enhance biological activity, particularly antitubercular effects (Manna & Agrawal, 2010; Sharma *et al.*, 2011; Shaharyar *et al.*, 2006). Moreover, 2AB has emerged as a promising candidate in antiviral drug development, as it acts as a ligand for the internal ribosome entry site (IRES) RNA of the hepatitis C virus (Rynearson *et al.*, 2014). In this study, we present the synthesis of a silver(I) coordination complex with 2AB, along with its crystal structure, supramolecular characteristics, and Hirshfeld surface analysis.



2. Structural commentary

The asymmetric unit of the synthesized complex consists of a single $[Ag(2AB)_2]NO_3{\cdot}(2AB)_2$ molecule. The central silver(I) atom is coordinated by two nitrogen donor atoms from 2-aminobenzoxazole ligands, forming an N_2 coordination set in a linear geometry while another two 2-aminobenzaxazole ligands and one nitrate anion remain uncoordinated (see Fig. 1). Each 2AB ligand binds in a monodentate fashion *via* its neutral nitrogen atom, exhibiting Ag—N bond lengths of 2.110 (5) and 2.116 (5) Å. The dihedral angle between the two oppositely coordinated 2-aminobenzoxazole ligands is 2.55 (7)°.

3. Supramolecular features

Hydrogen-bonding interactions occur between the components of the title complex. In particular, the amino groups of the two coordinated 2-aminobenzoxazole ligands interact with an oxygen and nitrogen atom of the nitrate anion through N—H⋯O and N—H⋯N interactions, while both of the uncoordinated 2-aminobenzoxazole ligands also form an N—H⋯O hydrogen bond with the nitrate anion (Table 1). Several N—H⋯N hydrogen bonds also occur. There is also an N—H⋯π interaction between the amino group and the six-membered aromatic ring of the 2-aminobenzoxazole ligand,

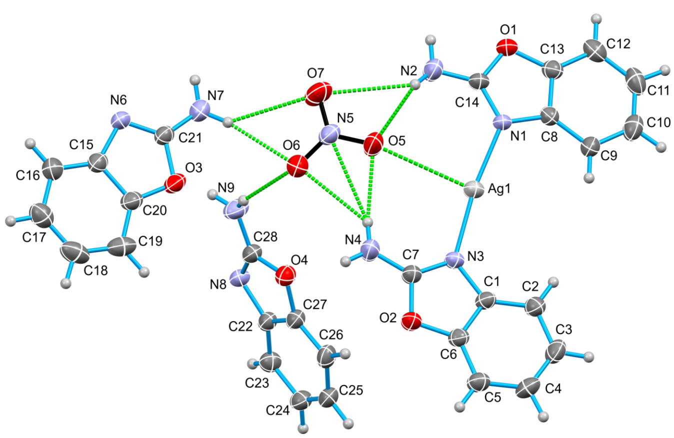


Figure 1
$[Ag(2AB)_2]NO_3{\cdot}(2AB)_2$ with displacement ellipsoids drawn at the 30% ellipsoid probability level showing the atom labelling. Hydrogen atoms are represented as small spheres with arbitrary radii and hydrogen bonds are indicated by dashed lines.

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

*Cg*11 is the centroid of the C22–C27 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2*A*⋯N6^{i}	0.84 (2)	2.15 (5)	2.915 (8)	151 (7)
N2—H2*B*⋯O5	0.83 (2)	2.15 (3)	2.937 (10)	158 (8)
N2—H2*B*⋯O7	0.83 (2)	2.65 (7)	3.271 (10)	133 (8)
N4—H4*A*⋯O5	0.85 (2)	2.14 (4)	2.937 (9)	157 (9)
N4—H4*A*⋯O6	0.85 (2)	2.46 (6)	3.084 (8)	131 (6)
N4—H4*A*⋯N5	0.85 (2)	2.64 (4)	3.434 (8)	156 (7)
N7—H7*A*⋯O7^{i}	0.84 (2)	2.17 (2)	3.012 (9)	175 (7)
N7—H7*B*⋯O6	0.85 (2)	2.24 (3)	3.069 (8)	165 (8)
N9—H9*A*⋯N8^{ii}	0.85 (2)	2.18 (3)	2.997 (9)	161 (9)
N9—H9*B*⋯O6	0.85 (2)	2.28 (5)	3.041 (10)	149 (9)
N4—H4*B*⋯*Cg*11^{iii}	0.85 (4)	2.58 (5)	3.403 (7)	162 (7)

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

N4—H4*B*⋯*Cg*11 (Fig. 2, Table 1). In addition both of the coordinated 2AB ligands participate in π–π interactions [*Cg*1⋯*Cg*7^{iv} = 3.584 (4) Å, dihedral angle = 6.7 (4)°; *Cg*2⋯*Cg*4^{v} = 3.609 (4) Å, dihedral angle = 2.5 (4)°; *Cg*4⋯*Cg*7^{iv} = 3.953 (4) Å, dihedral angle = 6.4 (4)°; where *Cg*1, *Cg*2, *Cg*4 and*Cg*7 are the centroids of the O1/C13/C8/N1/C14, O2/C6/C1/N3/C7, C8–13 and O3/C20/C15/N6/C21 rings, respectively; symmetry codes: (iv) $x, y-1, z$; (v) $1-x, -y, -z$]. η^2 Ag⋯π interactions are also observed involving adjacent carbon atoms of two phenyl rings. In the first ring, the Ag1⋯C8 and Ag1⋯C9 distances are 3.411 (6) and 3.186 (7) Å, respectively, while in the second ring, the Ag1⋯C16 and Ag1⋯C17 distances are 3.418 (9) and 3.345 (9) Å, respectively.

4. Hirshfeld Surface Analysis

A Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was performed and the two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were generated using *CrystalExplorer* (Spackman *et al.*, 2021) to quantify the intermolecular interactions (Fig. 3). The red spots on the HS indicate the presence of close intermolecular N—H⋯O and

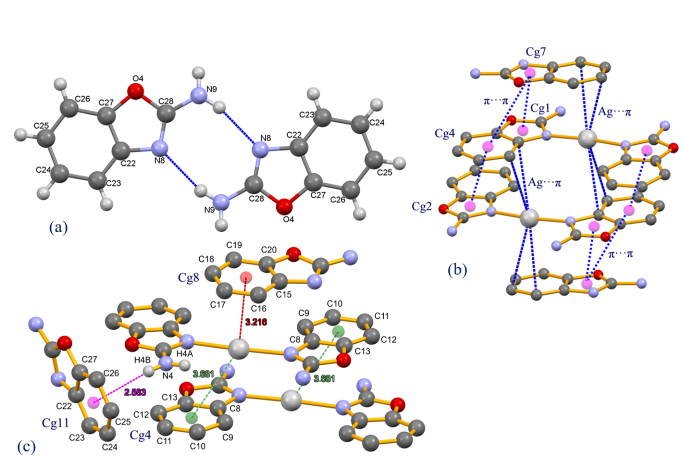


Figure 2
The packing of $[Ag(2AB)_2]NO_3{\cdot}(2AB)_2$ showing N—H⋯O, N—H⋯N, N—H⋯π, Ag⋯π, and π–π interactions.

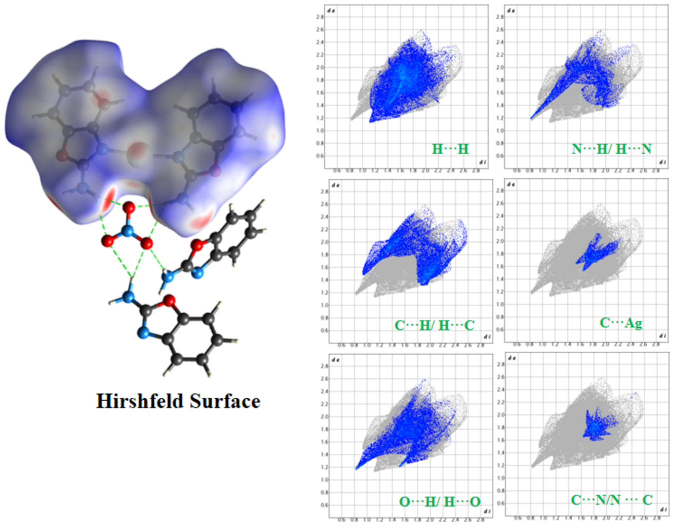


Figure 3
The Hirshfeld surface and corresponding two-dimensional fingerprint plots illustrating the contributions of different intermolecular contacts.

N—H···N interactions. The fingerprint plots shows that H···H (31.50%), C···H/H···C (19.60%), O···H/H···O (17.2%), N···H/H···N (9.60%), C···C (5.30%), C···N/N···C (4.40%), C···O/O···C (3.90%), and Ag···C/C···Ag (4.20%) are the major interactions contributing ~95.7% to the HS with minor interactions contributing less than 5%.

5. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.46, November 2024; Groom *et al.*, 2016) identified 18 crystal structures of 2-aminobenzoxazole (2AB) derivatives. Among them, only three structures (DIWPIM; Razzoqova *et al.*, 2023, MUYZEP; Razzoqova *et al.*, 2025, QALXIL; Decken & Gossage, 2005) were found for the 2-aminobenzoxazole moiety. Among these, one structure involves a zinc coordination complex (QALXIL), and two structures involve cadmium complexes (DIWPIM, MUYZEP). In the zinc complex QALXIL, the Zn^{II} centre adopts a distorted tetrahedral geometry, coordinating two 2AB ligands *via* their aromatic nitrogen atoms, along with two chloride ligands. The cadmium complex $[Cd(2AB)_2(CH3COO)_2]$ (DIWPIM) features a Cd^{II} ion coordinated by two 2AB ligands and two acetate ligands, binding in both monodentate and bidentate modes, resulting in a distorted octahedral coordination environment with an N_2O_4 donor set. In the complex $[Cd(2AB)_2(NO_3)_2]$ (MUYZEP), the cadmium(II) ion is coordinated by four 2AB ligands and two nitrate ions, forming a distorted octahedral geometry with an N_4O_2 coordination sphere.

6. Synthesis and crystallization

$AgNO_3$ (0.170 g, 1 mmol) and 2AB (0.268 g, 2 mmol) were dissolved separately in ethanol (5 ml), mixed together and stirred for 2 h. The obtained colourless solution was filtered and left for crystallization. Single crystals of the complex $[Ag(AB)_2](NO_3)(AB)_2$ suitable for X-ray analysis were obtained by slow evaporation of the solution over a period of 15d.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ag(C_7H_6N_2O)_2]NO_3{\cdot}2C_7H_6N_2O$
M_r	706.43
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	10.6356 (3), 11.2202 (5), 12.3475 (3)
α, β, γ (°)	92.459 (3), 94.903 (2), 98.682 (3)
V (Å^3)	1448.91 (8)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	6.13
Crystal size (mm)	0.11 × 0.09 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, H
Absorption correction	Multi-scan (*CrysAlis PRO* ; Rigaku OD, 2020)
T_{min}, T_{max}	0.332, 0.642
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14506, 5559, 4536
R_{int}	0.074
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.235, 1.12
No. of reflections	5559
No. of parameters	430
No. of restraints	12
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.62, −1.69

Computer programs: *CrysAlis PRO*(Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

7. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. All hydrogen atoms were located from difference-Fourier maps and refined isotropically; DFIX restraints were applied to the N—H bond lengths.

Acknowledgements

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supporting information

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Synthesis, crystal structure and Hirshfeld surface analysis of a coordination compound of silver nitrate with 2-aminobenzoxazole

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Computing details

Bis(2-aminobenzoxazole-κN)silver(I) nitrate–bis(2-aminobenzoxazole (1/2)

Crystal data

$[Ag(C_7H_6N_2O)_2]NO_3 \cdot 2C_7H_6N_2O$
$M_r = 706.43$
Triclinic, $P\bar{1}$
$a = 10.6356$ (3) Å
$b = 11.2202$ (5) Å
$c = 12.3475$ (3) Å
$\alpha = 92.459$ (3)°
$\beta = 94.903$ (2)°
$\gamma = 98.682$ (3)°
$V = 1448.91$ (8) Å^3
$Z = 2$
$F(000) = 716$
$D_x = 1.619$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 5786 reflections
$\theta = 3.6–71.3°$
$\mu = 6.13$ mm^{-1}
$T = 293$ K
Block, colourless
0.11 × 0.09 × 0.08 mm

Data collection

XtaLAB Synergy, Single source at home/near, H diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro ; Rigaku OD, 2020)
$T_{min} = 0.332$, $T_{max} = 0.642$
14506 measured reflections
5559 independent reflections
4536 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 71.6°$, $\theta_{min} = 3.6°$
$h = -13 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.235$
$S = 1.12$
5559 reflections
430 parameters
12 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1293P)^2 + 1.0923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.62$ e Å^{-3}
$\Delta\rho_{min} = -1.69$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.42768 (4)	0.08778 (4)	0.14010 (4)	0.0590 (2)
O1	0.1314 (4)	−0.0952 (4)	−0.0925 (4)	0.0592 (11)
O2	0.6801 (5)	0.3272 (4)	0.3700 (4)	0.0638 (12)
N1	0.3036 (5)	−0.0216 (5)	0.0205 (4)	0.0484 (11)
N2	0.1515 (7)	0.1029 (6)	−0.0354 (7)	0.0746 (17)
H2A	0.089 (6)	0.090 (7)	−0.083 (6)	0.090*
H2B	0.193 (7)	0.170 (4)	−0.016 (7)	0.090*
N3	0.5661 (5)	0.1799 (5)	0.2604 (4)	0.0512 (11)
N4	0.4995 (7)	0.3708 (6)	0.2761 (6)	0.0752 (18)
H4A	0.429 (5)	0.350 (6)	0.238 (7)	0.090*
H4B	0.523 (7)	0.445 (3)	0.297 (7)	0.090*
C1	0.6719 (6)	0.1359 (6)	0.3110 (5)	0.0521 (13)
C2	0.7103 (7)	0.0237 (6)	0.3025 (6)	0.0627 (16)
H2	0.662384	−0.040164	0.259658	0.075*
C3	0.8249 (8)	0.0118 (7)	0.3617 (7)	0.075 (2)
H3	0.854698	−0.061943	0.358073	0.090*
C4	0.8953 (7)	0.1069 (8)	0.4257 (7)	0.076 (2)
H4	0.972577	0.096078	0.462218	0.092*
C5	0.8547 (7)	0.2175 (7)	0.4370 (6)	0.0670 (17)
H5	0.900920	0.281153	0.481321	0.080*
C6	0.7402 (6)	0.2273 (6)	0.3778 (5)	0.0549 (14)
C7	0.5768 (6)	0.2919 (6)	0.2976 (5)	0.0543 (14)
C8	0.3061 (6)	−0.1432 (6)	−0.0033 (5)	0.0531 (14)
C9	0.3949 (7)	−0.2174 (6)	0.0292 (6)	0.0612 (16)
H9	0.467054	−0.188776	0.076390	0.073*
C10	0.3695 (9)	−0.3366 (7)	−0.0128 (7)	0.078 (2)
H10	0.425922	−0.389097	0.007756	0.093*
C11	0.2646 (10)	−0.3792 (7)	−0.0833 (8)	0.083 (2)
H11	0.251777	−0.459468	−0.109480	0.099*
C12	0.1768 (8)	−0.3055 (7)	−0.1166 (6)	0.0702 (19)
H12	0.105417	−0.333766	−0.164773	0.084*
C13	0.2017 (6)	−0.1878 (6)	−0.0740 (5)	0.0574 (14)
C14	0.1975 (6)	0.0008 (6)	−0.0326 (5)	0.0535 (14)
O3	0.2193 (5)	0.7580 (5)	0.2610 (4)	0.0659 (12)
N6	0.0707 (5)	0.8530 (5)	0.1741 (5)	0.0586 (13)
N7	0.0691 (7)	0.6442 (6)	0.1405 (5)	0.0709 (16)
H7A	0.013 (6)	0.643 (7)	0.088 (5)	0.085*
H7B	0.125 (6)	0.598 (6)	0.140 (6)	0.085*
C15	0.1506 (7)	0.9375 (7)	0.2480 (5)	0.0607 (16)

C16	0.1538 (8)	1.0573 (8)	0.2688 (7)	0.076 (2)
H16	0.095172	1.098802	0.232582	0.091*
C17	0.2475 (9)	1.1161 (9)	0.3460 (8)	0.083 (2)
H17	0.251395	1.198372	0.362370	0.100*
C18	0.3339 (9)	1.0549 (11)	0.3983 (7)	0.090 (3)
H18	0.394775	1.096878	0.450410	0.108*
C19	0.3348 (8)	0.9332 (10)	0.3771 (7)	0.085 (2)
H19	0.394560	0.892073	0.412464	0.101*
C20	0.2420 (7)	0.8774 (7)	0.3007 (6)	0.0622 (16)
C21	0.1159 (6)	0.7536 (6)	0.1864 (5)	0.0552 (14)
O4	0.2916 (4)	0.4227 (4)	0.4621 (4)	0.0620 (11)
N8	0.1235 (5)	0.4191 (5)	0.5619 (4)	0.0558 (12)
N9	0.1122 (7)	0.4853 (8)	0.3811 (6)	0.0777 (19)
H9A	0.040 (4)	0.509 (8)	0.382 (7)	0.093*
H9B	0.160 (6)	0.509 (8)	0.332 (6)	0.093*
C22	0.2243 (6)	0.3788 (5)	0.6238 (5)	0.0532 (13)
C23	0.2349 (7)	0.3414 (6)	0.7274 (6)	0.0624 (16)
H23	0.166796	0.337238	0.770247	0.075*
C24	0.3519 (7)	0.3095 (7)	0.7669 (6)	0.0674 (18)
H24	0.361718	0.285213	0.837797	0.081*
C25	0.4530 (7)	0.3132 (7)	0.7036 (6)	0.0672 (18)
H25	0.529411	0.291607	0.732625	0.081*
C26	0.4424 (7)	0.3483 (7)	0.5981 (7)	0.0649 (17)
H26	0.509288	0.350226	0.554071	0.078*
C27	0.3262 (6)	0.3804 (6)	0.5617 (6)	0.0566 (14)
C28	0.1690 (6)	0.4432 (6)	0.4704 (6)	0.0589 (15)
O5	0.3017 (6)	0.3107 (6)	0.0929 (6)	0.093 (2)
O6	0.2585 (6)	0.4664 (5)	0.1816 (5)	0.0798 (15)
O7	0.1249 (6)	0.3756 (7)	0.0546 (7)	0.109 (2)
N5	0.2266 (6)	0.3839 (6)	0.1100 (5)	0.0657 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0569 (4)	0.0592 (3)	0.0571 (3)	0.0089 (2)	−0.0119 (2)	−0.0049 (2)
O1	0.053 (2)	0.066 (3)	0.056 (2)	0.011 (2)	−0.0104 (19)	−0.004 (2)
O2	0.060 (3)	0.054 (2)	0.072 (3)	0.010 (2)	−0.019 (2)	−0.010 (2)
N1	0.046 (3)	0.051 (3)	0.047 (3)	0.011 (2)	−0.010 (2)	−0.004 (2)
N2	0.073 (4)	0.058 (3)	0.092 (5)	0.024 (3)	−0.012 (3)	0.000 (3)
N3	0.048 (3)	0.049 (3)	0.053 (3)	0.004 (2)	−0.011 (2)	−0.004 (2)
N4	0.069 (4)	0.065 (4)	0.091 (5)	0.026 (3)	−0.015 (3)	−0.015 (3)
C1	0.045 (3)	0.055 (3)	0.054 (3)	0.007 (2)	−0.006 (2)	0.006 (3)
C2	0.070 (4)	0.055 (4)	0.062 (4)	0.012 (3)	−0.008 (3)	0.003 (3)
C3	0.081 (5)	0.067 (4)	0.083 (5)	0.032 (4)	0.003 (4)	0.015 (4)
C4	0.060 (4)	0.089 (6)	0.081 (5)	0.023 (4)	−0.012 (4)	0.017 (4)
C5	0.059 (4)	0.068 (4)	0.070 (4)	0.008 (3)	−0.012 (3)	0.002 (3)
C6	0.055 (3)	0.057 (4)	0.051 (3)	0.009 (3)	−0.003 (3)	0.005 (3)
C7	0.051 (3)	0.052 (3)	0.058 (3)	0.008 (3)	−0.005 (3)	−0.001 (3)

C8	0.059 (4)	0.051 (3)	0.048 (3)	0.010 (3)	0.002 (3)	−0.001 (2)
C9	0.066 (4)	0.060 (4)	0.060 (4)	0.022 (3)	0.001 (3)	0.002 (3)
C10	0.091 (6)	0.065 (5)	0.086 (5)	0.032 (4)	0.016 (5)	0.016 (4)
C11	0.114 (7)	0.051 (4)	0.085 (6)	0.012 (4)	0.018 (5)	−0.009 (4)
C12	0.077 (5)	0.070 (5)	0.060 (4)	0.000 (4)	0.011 (3)	−0.010 (3)
C13	0.058 (4)	0.060 (4)	0.052 (3)	0.007 (3)	−0.001 (3)	0.000 (3)
C14	0.048 (3)	0.058 (3)	0.051 (3)	0.006 (3)	−0.010 (2)	−0.003 (3)
O3	0.062 (3)	0.081 (3)	0.059 (3)	0.030 (2)	−0.003 (2)	0.012 (2)
N6	0.053 (3)	0.067 (3)	0.058 (3)	0.022 (3)	−0.009 (2)	−0.004 (2)
N7	0.078 (4)	0.067 (4)	0.071 (4)	0.027 (3)	−0.003 (3)	0.005 (3)
C15	0.063 (4)	0.072 (4)	0.051 (3)	0.024 (3)	0.004 (3)	0.002 (3)
C16	0.076 (5)	0.078 (5)	0.074 (5)	0.023 (4)	0.001 (4)	−0.009 (4)
C17	0.083 (6)	0.077 (5)	0.084 (6)	0.002 (4)	0.006 (4)	−0.014 (4)
C18	0.068 (5)	0.120 (8)	0.072 (5)	−0.009 (5)	0.001 (4)	−0.021 (5)
C19	0.064 (5)	0.119 (8)	0.066 (5)	0.008 (5)	−0.009 (4)	0.016 (5)
C20	0.058 (4)	0.079 (5)	0.051 (3)	0.020 (3)	−0.002 (3)	0.006 (3)
C21	0.050 (3)	0.067 (4)	0.052 (3)	0.021 (3)	0.002 (3)	0.004 (3)
O4	0.060 (3)	0.073 (3)	0.057 (2)	0.023 (2)	0.006 (2)	0.003 (2)
N8	0.047 (3)	0.063 (3)	0.056 (3)	0.013 (2)	−0.007 (2)	0.000 (2)
N9	0.075 (4)	0.103 (5)	0.060 (4)	0.031 (4)	−0.002 (3)	0.018 (3)
C22	0.049 (3)	0.050 (3)	0.060 (3)	0.012 (2)	−0.004 (3)	0.001 (3)
C23	0.056 (4)	0.064 (4)	0.065 (4)	0.008 (3)	−0.001 (3)	0.001 (3)
C24	0.074 (4)	0.064 (4)	0.064 (4)	0.018 (3)	−0.011 (3)	0.007 (3)
C25	0.067 (4)	0.066 (4)	0.071 (4)	0.028 (3)	−0.010 (3)	0.000 (3)
C26	0.054 (4)	0.067 (4)	0.078 (5)	0.023 (3)	0.009 (3)	0.000 (3)
C27	0.057 (4)	0.052 (3)	0.062 (4)	0.016 (3)	−0.004 (3)	0.003 (3)
C28	0.058 (4)	0.058 (4)	0.061 (4)	0.017 (3)	−0.009 (3)	0.003 (3)
O5	0.080 (4)	0.077 (4)	0.123 (5)	0.039 (3)	−0.028 (3)	−0.023 (3)
O6	0.089 (4)	0.080 (4)	0.074 (3)	0.033 (3)	−0.005 (3)	−0.005 (3)
O7	0.077 (4)	0.098 (5)	0.145 (6)	0.023 (3)	−0.045 (4)	−0.002 (4)
N5	0.060 (3)	0.066 (4)	0.072 (4)	0.020 (3)	−0.006 (3)	0.010 (3)

Geometric parameters (Å, º)

Ag1—N1	2.110 (5)	O3—C20	1.386 (10)
Ag1—N3	2.116 (5)	N6—C21	1.289 (8)
O1—C14	1.347 (8)	N6—C15	1.415 (9)
O1—C13	1.384 (8)	N7—C21	1.335 (10)
O2—C7	1.353 (8)	N7—H7A	0.84 (2)
O2—C6	1.375 (8)	N7—H7B	0.85 (2)
N1—C14	1.319 (8)	C15—C16	1.352 (11)
N1—C8	1.388 (8)	C15—C20	1.397 (9)
N2—C14	1.313 (9)	C16—C17	1.386 (12)
N2—H2A	0.84 (2)	C16—H16	0.9300
N2—H2B	0.83 (2)	C17—C18	1.365 (14)
N3—C7	1.305 (8)	C17—H17	0.9300
N3—C1	1.406 (8)	C18—C19	1.382 (15)
N4—C7	1.316 (9)	C18—H18	0.9300

N4—H4A	0.85 (2)	C19—C20	1.363 (11)
N4—H4B	0.86 (2)	C19—H19	0.9300
C1—C6	1.363 (9)	O4—C28	1.370 (8)
C1—C2	1.383 (10)	O4—C27	1.378 (8)
C2—C3	1.394 (10)	N8—C28	1.289 (9)
C2—H2	0.9300	N8—C22	1.405 (7)
C3—C4	1.382 (12)	N9—C28	1.349 (9)
C3—H3	0.9300	N9—H9A	0.85 (2)
C4—C5	1.380 (11)	N9—H9B	0.85 (2)
C4—H4	0.9300	C22—C23	1.364 (9)
C5—C6	1.388 (9)	C22—C27	1.379 (9)
C5—H5	0.9300	C23—C24	1.400 (10)
C8—C13	1.369 (10)	C23—H23	0.9300
C8—C9	1.395 (9)	C24—C25	1.378 (11)
C9—C10	1.393 (11)	C24—H24	0.9300
C9—H9	0.9300	C25—C26	1.378 (11)
C10—C11	1.367 (13)	C25—H25	0.9300
C10—H10	0.9300	C26—C27	1.383 (9)
C11—C12	1.385 (13)	C26—H26	0.9300
C11—H11	0.9300	O5—N5	1.253 (8)
C12—C13	1.380 (10)	O6—N5	1.240 (8)
C12—H12	0.9300	O7—N5	1.218 (8)
O3—C21	1.367 (8)		

N1—Ag1—N3	172.85 (18)	N1—C14—O1	113.8 (5)
C14—O1—C13	104.7 (5)	C21—O3—C20	103.4 (5)
C7—O2—C6	104.8 (5)	C21—N6—C15	104.2 (5)
C14—N1—C8	105.1 (5)	C21—N7—H7A	115 (6)
C14—N1—Ag1	129.1 (4)	C21—N7—H7B	112 (6)
C8—N1—Ag1	124.9 (4)	H7A—N7—H7B	121 (4)
C14—N2—H2A	105 (6)	C16—C15—C20	120.3 (7)
C14—N2—H2B	125 (6)	C16—C15—N6	131.9 (7)
H2A—N2—H2B	125 (4)	C20—C15—N6	107.8 (6)
C7—N3—C1	105.3 (5)	C15—C16—C17	117.8 (8)
C7—N3—Ag1	127.5 (4)	C15—C16—H16	121.1
C1—N3—Ag1	127.0 (4)	C17—C16—H16	121.1
C7—N4—H4A	121 (5)	C18—C17—C16	120.8 (9)
C7—N4—H4B	120 (5)	C18—C17—H17	119.6
H4A—N4—H4B	119 (4)	C16—C17—H17	119.6
C6—C1—C2	121.3 (6)	C17—C18—C19	122.7 (8)
C6—C1—N3	107.6 (5)	C17—C18—H18	118.6
C2—C1—N3	131.2 (6)	C19—C18—H18	118.6
C1—C2—C3	116.3 (7)	C20—C19—C18	115.3 (8)
C1—C2—H2	121.9	C20—C19—H19	122.3
C3—C2—H2	121.9	C18—C19—H19	122.3
C4—C3—C2	121.5 (7)	C19—C20—O3	129.0 (7)
C4—C3—H3	119.2	C19—C20—C15	123.0 (8)
C2—C3—H3	119.2	O3—C20—C15	108.0 (6)

C5—C4—C3	122.1 (7)	N6—C21—N7	128.0 (6)
C5—C4—H4	118.9	N6—C21—O3	116.5 (6)
C3—C4—H4	118.9	N7—C21—O3	115.3 (6)
C4—C5—C6	115.4 (7)	C28—O4—C27	103.6 (5)
C4—C5—H5	122.3	C28—N8—C22	104.0 (5)
C6—C5—H5	122.3	C28—N9—H9A	122 (6)
C1—C6—O2	108.6 (5)	C28—N9—H9B	117 (6)
C1—C6—C5	123.3 (6)	H9A—N9—H9B	118 (4)
O2—C6—C5	128.0 (6)	C23—C22—C27	119.4 (6)
N3—C7—N4	128.5 (6)	C23—C22—N8	131.8 (6)
N3—C7—O2	113.7 (5)	C27—C22—N8	108.7 (5)
N4—C7—O2	117.8 (6)	C22—C23—C24	117.7 (7)
C13—C8—N1	108.4 (6)	C22—C23—H23	121.2
C13—C8—C9	120.3 (6)	C24—C23—H23	121.2
N1—C8—C9	131.3 (6)	C25—C24—C23	121.8 (7)
C10—C9—C8	116.4 (7)	C25—C24—H24	119.1
C10—C9—H9	121.8	C23—C24—H24	119.1
C8—C9—H9	121.8	C26—C25—C24	121.0 (6)
C11—C10—C9	122.3 (7)	C26—C25—H25	119.5
C11—C10—H10	118.9	C24—C25—H25	119.5
C9—C10—H10	118.9	C25—C26—C27	115.9 (7)
C10—C11—C12	121.5 (7)	C25—C26—H26	122.0
C10—C11—H11	119.2	C27—C26—H26	122.0
C12—C11—H11	119.2	O4—C27—C22	107.9 (5)
C13—C12—C11	116.0 (8)	O4—C27—C26	127.9 (6)
C13—C12—H12	122.0	C22—C27—C26	124.2 (6)
C11—C12—H12	122.0	N8—C28—N9	129.0 (6)
C8—C13—C12	123.5 (7)	N8—C28—O4	115.8 (5)
C8—C13—O1	108.0 (6)	N9—C28—O4	115.2 (6)
C12—C13—O1	128.5 (7)	O7—N5—O6	120.7 (7)
N2—C14—N1	128.5 (6)	O7—N5—O5	120.0 (7)
N2—C14—O1	117.7 (6)	O6—N5—O5	119.3 (6)

C7—N3—C1—C6	0.5 (7)	C8—N1—C14—O1	−2.1 (7)
Ag1—N3—C1—C6	176.1 (4)	Ag1—N1—C14—O1	−171.0 (4)
C7—N3—C1—C2	−179.8 (7)	C13—O1—C14—N2	179.8 (7)
Ag1—N3—C1—C2	−4.2 (11)	C13—O1—C14—N1	1.0 (7)
C6—C1—C2—C3	−2.9 (11)	C21—N6—C15—C16	177.0 (8)
N3—C1—C2—C3	177.4 (7)	C21—N6—C15—C20	0.1 (7)
C1—C2—C3—C4	0.4 (12)	C20—C15—C16—C17	−2.1 (12)
C2—C3—C4—C5	1.9 (13)	N6—C15—C16—C17	−178.6 (7)
C3—C4—C5—C6	−1.5 (12)	C15—C16—C17—C18	0.5 (13)
C2—C1—C6—O2	−179.9 (6)	C16—C17—C18—C19	0.9 (14)
N3—C1—C6—O2	−0.2 (7)	C17—C18—C19—C20	−0.7 (13)
C2—C1—C6—C5	3.4 (11)	C18—C19—C20—O3	179.0 (8)
N3—C1—C6—C5	−176.9 (7)	C18—C19—C20—C15	−0.9 (12)
C7—O2—C6—C1	−0.2 (7)	C21—O3—C20—C19	−179.6 (7)
C7—O2—C6—C5	176.3 (7)	C21—O3—C20—C15	0.3 (7)

C4—C5—C6—C1	−1.1 (11)	C16—C15—C20—C19	2.3 (12)
C4—C5—C6—O2	−177.1 (7)	N6—C15—C20—C19	179.6 (7)
C1—N3—C7—N4	−178.6 (8)	C16—C15—C20—O3	−177.6 (7)
Ag1—N3—C7—N4	5.9 (11)	N6—C15—C20—O3	−0.3 (8)
C1—N3—C7—O2	−0.7 (8)	C15—N6—C21—N7	175.1 (7)
Ag1—N3—C7—O2	−176.2 (4)	C15—N6—C21—O3	0.1 (8)
C6—O2—C7—N3	0.6 (8)	C20—O3—C21—N6	−0.2 (8)
C6—O2—C7—N4	178.7 (7)	C20—O3—C21—N7	−175.9 (6)
C14—N1—C8—C13	2.2 (7)	C28—N8—C22—C23	179.3 (7)
Ag1—N1—C8—C13	171.8 (4)	C28—N8—C22—C27	−0.7 (7)
C14—N1—C8—C9	179.7 (7)	C27—C22—C23—C24	1.8 (10)
Ag1—N1—C8—C9	−10.7 (10)	N8—C22—C23—C24	−178.2 (7)
C13—C8—C9—C10	−0.9 (10)	C22—C23—C24—C25	−1.2 (11)
N1—C8—C9—C10	−178.1 (7)	C23—C24—C25—C26	−0.2 (12)
C8—C9—C10—C11	0.9 (12)	C24—C25—C26—C27	0.8 (11)
C9—C10—C11—C12	−0.3 (14)	C28—O4—C27—C22	−0.5 (7)
C10—C11—C12—C13	−0.3 (12)	C28—O4—C27—C26	−178.4 (7)
N1—C8—C13—C12	178.2 (7)	C23—C22—C27—O4	−179.3 (6)
C9—C8—C13—C12	0.3 (11)	N8—C22—C27—O4	0.8 (7)
N1—C8—C13—O1	−1.7 (7)	C23—C22—C27—C26	−1.3 (10)
C9—C8—C13—O1	−179.5 (6)	N8—C22—C27—C26	178.8 (6)
C11—C12—C13—C8	0.3 (11)	C25—C26—C27—O4	177.5 (7)
C11—C12—C13—O1	−179.9 (7)	C25—C26—C27—C22	−0.1 (11)
C14—O1—C13—C8	0.4 (7)	C22—N8—C28—N9	−180.0 (8)
C14—O1—C13—C12	−179.4 (7)	C22—N8—C28—O4	0.5 (8)
C8—N1—C14—N2	179.3 (8)	C27—O4—C28—N8	0.0 (8)
Ag1—N1—C14—N2	10.4 (11)	C27—O4—C28—N9	−179.6 (7)

Hydrogen-bond geometry (Å, º)

*Cg*11 is the centroid of the C22–C27 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N6^{i}	0.84 (2)	2.15 (5)	2.915 (8)	151 (7)
N2—H2*B*···O5	0.83 (2)	2.15 (3)	2.937 (10)	158 (8)
N2—H2*B*···O7	0.83 (2)	2.65 (7)	3.271 (10)	133 (8)
N4—H4*A*···O5	0.85 (2)	2.14 (4)	2.937 (9)	157 (9)
N4—H4*A*···O6	0.85 (2)	2.46 (6)	3.084 (8)	131 (6)
N4—H4*A*···N5	0.85 (2)	2.64 (4)	3.434 (8)	156 (7)
N7—H7*A*···O7^{i}	0.84 (2)	2.17 (2)	3.012 (9)	175 (7)
N7—H7*B*···O6	0.85 (2)	2.24 (3)	3.069 (8)	165 (8)
N9—H9*A*···N8^{ii}	0.85 (2)	2.18 (3)	2.997 (9)	161 (9)
N9—H9*B*···O6	0.85 (2)	2.28 (5)	3.041 (10)	149 (9)
N4—H4*B*···*Cg*11^{iii}	0.85 (4)	2.58 (5)	3.403 (7)	162 (7)

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

pi-pi interactions

Cg(i)	Cg(j)	distance (Å)	dihedra anglel (°)
1	7^{iv}	3.584 (4)	6.7 (4)
2	4^{v}	3.609 (4)	2.5 (4)
4	7^{iv}	3.953 (4)	6.4 (4)

Cg1 = O1-C13-C8-N1-C14; Cg2 = O2-C6-C1-N3-C7; Cg3 = C1-C6; Cg4 = C8-13; Cg7 = O3-C20-C15-N6-C21; Cg8 = C15-C20; Cg10 = O4-C27-C22-N8-C28; Cg11 = C22 -C27; Symmetry codes: (iv) x, y-1, z; (v) 1-x, -y, -z.