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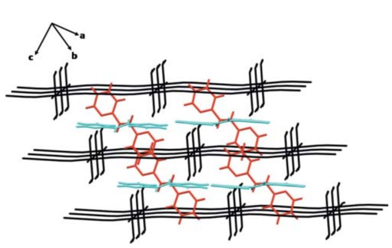

Crystal structure of a two-dimensional grid-type iron(II) coordination polymer: poly[[diaquatetra-μ-cyanido-diargentate(I)iron(II)] *trans*-1,2-bis(pyridin-2-yl)ethylene disolvate]

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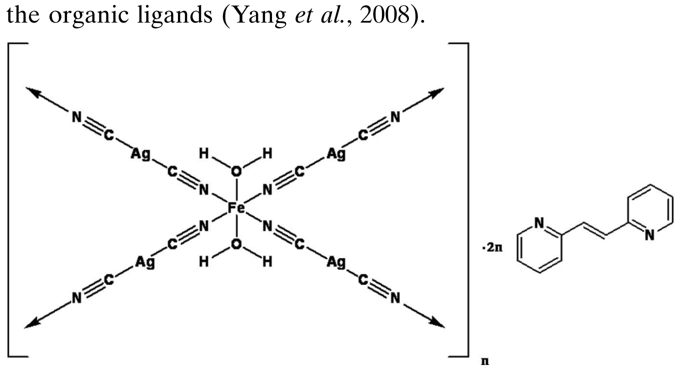
In the title compound, $\{[Ag_2Fe(CN)_4(H_2O)_2]\cdot 2C_{12}H_{10}N_2\}_n$, the asymmetric unit contains one Fe^{II} cation, two water molecules, two dicyanidoargentate(I) anions and two uncoordinating 1,2-bis(pyridin-2-yl)ethylene (2,2′-bpe) molecules. Each Fe^{II} atom is six-coordinated in a nearly regular octahedral geometry by four N atoms from dicyanidoargentate(I) bridges and two coordinating water molecules. The Fe^{II} atoms are bridged by dicyanidoargentate(I) units to give a two-dimensional layer with square-grid spaces. The intergrid spaces with interlayer distance of 6.550 (2) Å are occupied by 2,2′-bpe guest molecules which form O—H···N hydrogen bonds to the host layers. This leads to an extended three-dimensional supramolecular architecture. The structure of the title compound is compared with some related compounds containing dicyanidoargentate(I) ligands and N-donor organic co-ligands.

1. Chemical context

Metal–organic frameworks (MOFs) have attracted much attention because of their versatile topologies and dimensions. These structural properties lead to potential interesting applications in the filed of magnetism, sensing, porous materials and catalysis (Biswas *et al.*, 2014; Horike *et al.*, 2008; Sanda *et al.*, 2013). Structural diversity in MOFs can occur as a result of various preparation methods. However, supramolecular chemistry and topologies of MOFs are rather controlled by the nature of the metal ions and the structure of the organic ligands (Yang *et al.*, 2008).



One-, two- and three-dimensional frameworks containing dicyanidoargentate(I) and N-donor linkers such as pyrazine, 4,4′-bpy and 4,4′-bpe [bpy is bipyridineand bpe is 1,2-bis(4-pyridyl)ethylene] ligands have been studied (Soma &

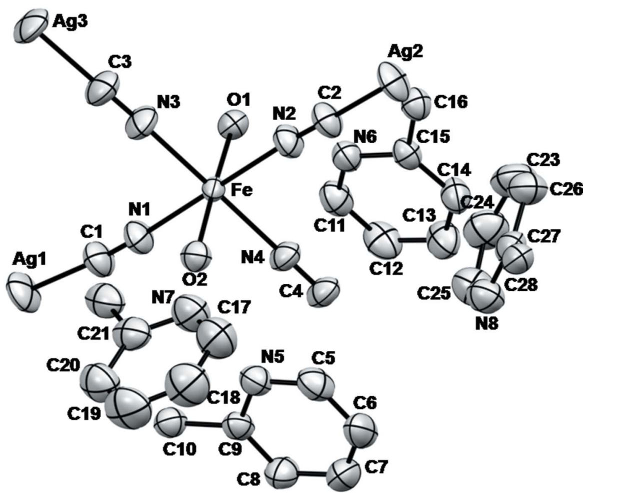


Figure 1
A view of the asymmetric unit in (I), showing displacement ellipsoids at the 50% probability level and the atom-numbering scheme. H atoms have been omitted for clarity.

Iwamoto, 1996; Munoz *et al.*, 2007; Dong *et al.*, 2003). Whereas 4,4′-bpe appears to be somewhat ubiquitous in cyanido compounds, its cousin 2,2′-bpe is not very often used, which led us to prepare a dicyanidoargentate(I) compound with a 2,2′-bpe ligand. In this communication, we report the synthesis and crystal structure of a three-dimensional supramolecular framework of $\{[Ag_2Fe(CN)_4(H_2O)_2]\cdot 2C_{12}H_{10}N_2\}_n$, (I).

2. Structural commentary

The asymmetric unit consists of one Fe^{II} atom, two dicyanidoargentate(I) ligands, two water molecules and two uncoordinating 2,2′-bpe molecules (Fig. 1). Ag1 and Ag2 are situated on inversion centres. The dicyanidoargentate(I) ligands link Fe^{II} atoms into an infinite two-dimensional layer network with a nearly square-grid geometry of 10.66 × 10.64 $Å^2$ (Fig. 2). The Fe^{II} ion is six-cooordinated (Table 1) in a nearly regular octahedral geometry by four N atoms from four dicyanidoargentate(I) ligands and two water molecules.

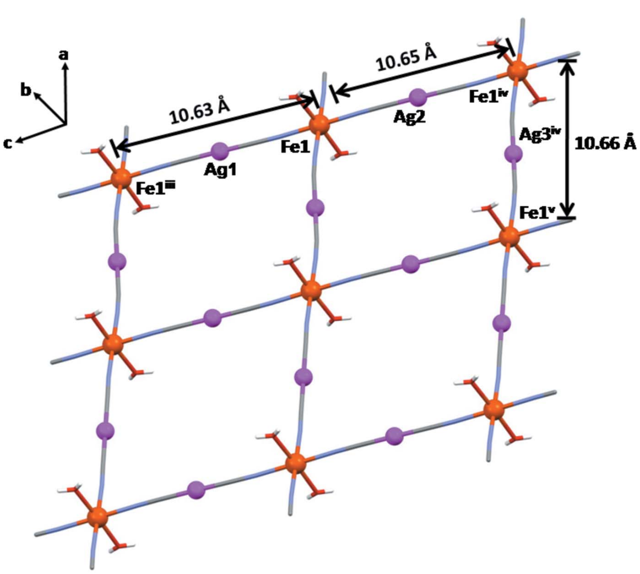


Figure 2
A view of the square grid of (I) in the *ac* plane; the 2,2′-bpe molecules have been omitted. [Symmetry codes: (iii) $-x + 1, -y + 2, z$; (iv) $-x, -y + 1, -z + 1$; (v) $-x + 1, -y, -z + 1$.]

Table 1
Selected bond lengths (Å).

Fe—O1	2.1365 (15)	Fe—N4	2.1489 (16)
Fe—O2	2.1392 (16)	Fe—N2	2.1522 (16)
Fe—N1	2.1440 (17)	Fe—N3	2.1539 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H2*W*···N5	0.76 (3)	2.07 (3)	2.829 (2)	174 (2)
O2—H4*W*···N6	0.73 (3)	2.09 (3)	2.823 (3)	174 (3)
O1—H1*W*···N7^{i}	0.75 (3)	2.14 (3)	2.870 (3)	164
O2—H3*W*···N8^{ii}	0.74 (3)	2.15 (3)	2.868 (3)	162

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

3. Supramolecular features

Four independent 2,2′-bpe molecules are located between adjacent grid layers of which two are parallel (blue) to the grid layers and two non-parallel (red) (Fig. 3). The interlayer distance is 6.550 (2) Å. The two parallel 2,2′-bpe ligands form hydrogen bonds (Table 2) to the host layer (O1—H2*W*···N5 = 2.07 Å and O2–H4*W*···N6 = 2.09 Å) (Fig. 4*a*), while the other two arrange themselves across the host layer to form also hydrogen bonds (O1—H1*W*···N7 = 2.14 Å and O2—H3*W*···N8 = 2.15 Å) (Fig. 4*b*) to the host layers. These hydrogen bonds generate an extended three-dimensional supramolecular framework.

4. Database survey

The two-dimensional structure of (I) was found to be different from other closely related compounds. In the structure of $[Cd(imH)_4[Ag(CN)_2]_2]_n$ (imH = imidazole), a one-dimen-

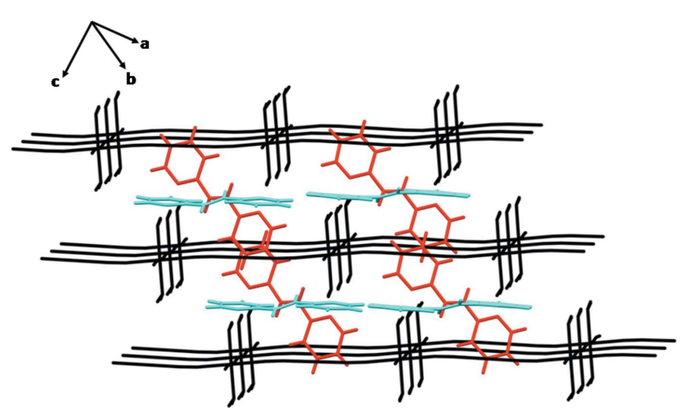


Figure 3
2,2′-Bpe in parallel (blue) and non-parallel (red) fashion between adjacent layers.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ag_2Fe(CN)_4(H_2O)_2]\cdot 2C_{12}H_{10}N_2$
M_r	776.14
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	9.2078 (4), 9.8558 (5), 18.9029 (9)
α, β, γ (°)	77.667 (1), 77.507 (1), 67.900 (1)
V (Å^3)	1535.11 (13)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.77
Crystal size (mm)	0.43 × 0.11 × 0.09
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.684, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	21143, 7389, 5865
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.073, 1.03
No. of reflections	7389
No. of parameters	389
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.37

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

sional chain *via* bridging dicyanidoargentate(I) is found, while all imidazole molecules act as a terminal ligand (Takayoshi & Toschitake, 1996). In addition, the two-dimensional framework of $[Fe(3\text{-}Fpy)_2[Ag(CN)_2]_2]_n$ (3-Fpy = 3-fluoropyridine) consists of four cyanide moieties occupying the equatorial positions generating a square grid-type structure similar to that of the title compound, while the axial positions are occupied by two terminal 3-Fpy ligands instead of two water molecules in (I) (Munoz *et al.*, 2007). When the terminal ligands such as imH and 3-Fpy are replaced by N-donor linkers such as pyrazine, 4,4′-bpy and 4,4′-bpe, three-dimensional interpenetrating frameworks are obtained, as in $\{[Fe(pz)[Ag(CN)_2]_2].pz\}_n$ (pz = pyrazine), $[Mn(4,4'\text{-}bpy)_2\text{-}[Ag(CN)_2]_2]_n$, $[Fe(4,4'\text{-}bpy)_2[Ag(CN)_2]_2]_n$ and $[Fe(bpe)_2\text{-}[Ag(CN)_2]_2]_n$ (Niel *et al.*, 2002; Dong *et al.*, 2003). The last compound contains bpe bridges, while in the title compound 2,2′-bpe behaves as the organic guest molecules in the lattice. This could be the result of the difference in the N-donor position.

5. Synthesis and crystallization

An aqueous solution (5 ml) of $K[Ag(CN)_2]$ (0.0995 g, 0.5 mmol) was added dropwise to an MeOH–H_2O mixed solution (1:1 v/v, 10 ml) of $(NH_4)_2[Fe(SO_4)_2]\cdot 6H_2O$ (0.0980 g, 0.25 mmol) and 2,2′-bpe (0.0911 g, 0.5 mmol) at room temperature. After filtration and slow evaporation for 1 d, yellow crystals were obtained.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically and included as riding atoms, with aromatic C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in difference Fourier maps and refined isotropically.

Acknowledgements

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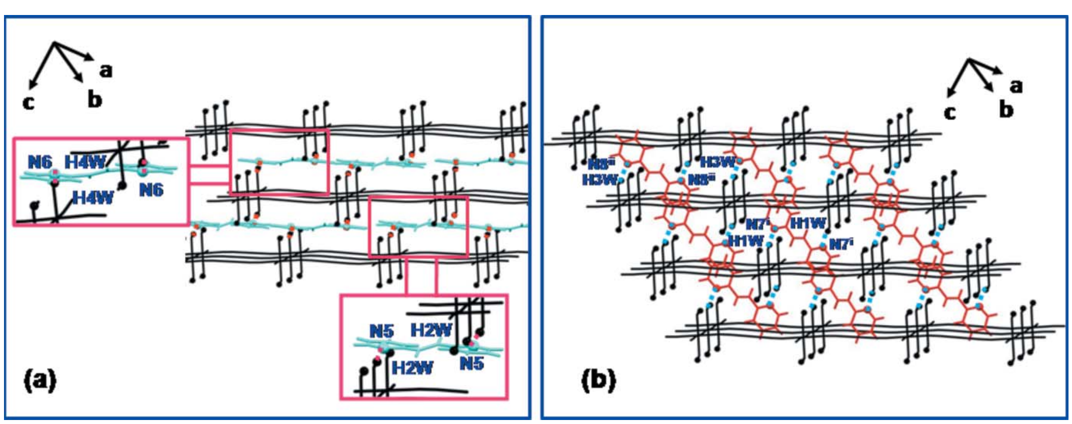

Figure 4
A fragment of the three-dimensional supramolecular framework *via* N···H—O hydrogen-bonding interactions between (*a*) parallel 2,2′-bpe and coordinating water molecules (dashed lines), and (*b*) non-parallel 2,2′-bpe and coordinating water molecules (dashed lines). [Symmetry codes: (i) $x - 1, y, z$; (ii) $x, y + 1, z$.]

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Crystal structure of a two-dimensional grid-type iron(II) coordination polymer: poly[[diaquatetra-*μ*-cyanido-diargentate(I)iron(II)] *trans*-1,2-bis(pyridin-2-yl)ethylene disolvate]

Jintana Othong, Nanthawat Wannarit, Chaveng Pakawatchai and Sujittra Youngme

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SMART* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Poly[[diaquatetra-*μ*-cyanido-diargentate(I)iron(II)] bis[*trans*-1,2-bis(pyridin-2-yl)ethylene]]

Crystal data

$[Ag_2Fe(CN)_4(H_2O)_2]\cdot 2C_{12}H_{10}N_2$
M_r = 776.14
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.2078 (4) Å
b = 9.8558 (5) Å
c = 18.9029 (9) Å
α = 77.667 (1)°
β = 77.507 (1)°
γ = 67.900 (1)°
V = 1535.11 (13) Å^3
Z = 2
$F(000)$ = 768
776.14
D_x = 1.679 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 1.77 mm^{-1}
T = 293 K
Block, yellow
0.43 × 0.11 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.684, T_{max} = 1.000
21143 measured reflections
7389 independent reflections
5865 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.0°, θ_{min} = 1.1°
$h = -12\rightarrow12$
$k = -13\rightarrow13$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 1.03
7389 reflections
389 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.1941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ag3	−0.235709 (19)	1.239825 (17)	0.249406 (10)	0.06308 (7)
Ag2	0.0000	0.5000	0.5000	0.05956 (8)
Ag1	0.5000	1.0000	0.0000	0.06538 (9)
Fe	0.26653 (3)	0.74083 (2)	0.251508 (12)	0.02989 (7)
O1	0.15978 (19)	0.64325 (19)	0.19630 (8)	0.0437 (3)
O2	0.3821 (2)	0.83190 (18)	0.30581 (9)	0.0440 (3)
N3	0.0604 (2)	0.9394 (2)	0.25270 (11)	0.0562 (5)
N2	0.1689 (2)	0.64872 (19)	0.35630 (9)	0.0476 (4)
N1	0.3633 (2)	0.83204 (19)	0.14683 (9)	0.0497 (4)
N4	0.4711 (2)	0.54179 (18)	0.24955 (10)	0.0453 (4)
N5	0.3585 (2)	0.37522 (19)	0.14391 (9)	0.0472 (4)
N6	0.6565 (2)	0.62355 (18)	0.36001 (9)	0.0446 (4)
N7	0.9350 (3)	0.7412 (3)	0.09581 (12)	0.0717 (6)
C26	0.2054 (3)	0.1175 (3)	0.52221 (14)	0.0675 (7)
H26	0.1402	0.1178	0.5673	0.081*
C3	−0.0459 (3)	1.0458 (3)	0.25155 (14)	0.0618 (6)
C2	0.1135 (3)	0.5943 (2)	0.40815 (11)	0.0508 (5)
C1	0.4140 (3)	0.8860 (3)	0.09364 (11)	0.0541 (5)
C4	0.5760 (2)	0.4344 (2)	0.24875 (12)	0.0494 (5)
C5	0.3629 (3)	0.2536 (3)	0.19190 (12)	0.0577 (6)
H5	0.2794	0.2601	0.2304	0.069*
C6	0.4827 (3)	0.1197 (3)	0.18812 (13)	0.0653 (7)
H6	0.4789	0.0369	0.2220	0.078*
C7	0.6076 (3)	0.1114 (3)	0.13335 (13)	0.0676 (7)
H7	0.6930	0.0232	0.1303	0.081*
C8	0.6063 (3)	0.2340 (2)	0.08276 (12)	0.0569 (6)
H8	0.6908	0.2295	0.0450	0.068*
C9	0.4787 (2)	0.3644 (2)	0.08807 (10)	0.0422 (4)
C10	0.4628 (2)	0.4983 (2)	0.03421 (11)	0.0458 (5)
H10	0.3953	0.5880	0.0492	0.055*
C11	0.7884 (3)	0.6068 (2)	0.31163 (11)	0.0534 (5)

H11	0.7929	0.6865	0.2756	0.064*
C12	0.9174 (3)	0.4796 (3)	0.31178 (13)	0.0596 (6)
H12	1.0074	0.4736	0.2771	0.072*
C13	0.9117 (3)	0.3612 (3)	0.36401 (13)	0.0610 (6)
H13	0.9963	0.2719	0.3646	0.073*
C14	0.7776 (3)	0.3769 (2)	0.41567 (12)	0.0516 (5)
H14	0.7718	0.2984	0.4521	0.062*
C15	0.6523 (2)	0.5092 (2)	0.41323 (10)	0.0405 (4)
C16	0.5075 (2)	0.5375 (2)	0.46672 (11)	0.0442 (5)
H16	0.4180	0.6149	0.4528	0.053*
C17	0.8716 (4)	0.6370 (3)	0.10434 (16)	0.0836 (8)
H17	0.8639	0.5809	0.1504	0.100*
C18	0.8173 (4)	0.6069 (4)	0.05021 (19)	0.0864 (9)
H18	0.7721	0.5338	0.0590	0.104*
C19	0.8315 (4)	0.6881 (4)	−0.01761 (19)	0.0913 (10)
H19	0.7987	0.6689	−0.0564	0.110*
C20	0.8947 (3)	0.7982 (3)	−0.02814 (15)	0.0754 (7)
H20	0.9050	0.8541	−0.0741	0.091*
C21	0.9428 (3)	0.8251 (3)	0.03048 (14)	0.0603 (6)
C22	1.0045 (3)	0.9443 (3)	0.02706 (13)	0.0649 (7)
H22	1.0535	0.9411	0.0658	0.078*
C23	0.3203 (4)	0.1815 (3)	0.50884 (18)	0.0817 (9)
H23	0.3330	0.2257	0.5448	0.098*
C24	0.4143 (4)	0.1796 (3)	0.44306 (17)	0.0782 (8)
H24	0.4900	0.2252	0.4321	0.094*
C25	0.3943 (3)	0.1080 (3)	0.39311 (15)	0.0762 (7)
H25	0.4617	0.1032	0.3486	0.091*
N8	0.2859 (2)	0.0455 (2)	0.40410 (11)	0.0627 (5)
C27	0.1880 (3)	0.0527 (2)	0.46773 (12)	0.0534 (5)
C28	0.0623 (3)	−0.0088 (2)	0.47413 (12)	0.0574 (6)
H28	0.0714	−0.0651	0.4386	0.069*
H1W	0.096 (3)	0.684 (2)	0.1727 (12)	0.044 (7)*
H2W	0.211 (3)	0.574 (3)	0.1795 (13)	0.062 (8)*
H3W	0.339 (3)	0.887 (3)	0.3313 (13)	0.053 (8)*
H4W	0.450 (3)	0.779 (3)	0.3230 (14)	0.062 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag3	0.04673 (11)	0.03995 (10)	0.08458 (15)	0.01369 (7)	−0.01787 (10)	−0.01697 (9)
Ag2	0.06824 (17)	0.07681 (18)	0.03192 (12)	−0.03820 (14)	0.00292 (11)	0.00933 (11)
Ag1	0.08051 (19)	0.07607 (18)	0.03474 (13)	−0.03990 (15)	0.00655 (12)	0.01030 (12)
Fe	0.02927 (13)	0.02553 (12)	0.02578 (13)	−0.00351 (10)	0.00002 (10)	−0.00020 (9)
O1	0.0401 (8)	0.0444 (8)	0.0442 (8)	−0.0085 (7)	−0.0104 (7)	−0.0089 (7)
O2	0.0484 (9)	0.0357 (8)	0.0442 (9)	−0.0082 (7)	−0.0085 (7)	−0.0083 (7)
N3	0.0452 (10)	0.0412 (10)	0.0621 (12)	0.0063 (8)	−0.0073 (9)	−0.0065 (9)
N2	0.0514 (10)	0.0524 (10)	0.0336 (9)	−0.0206 (8)	0.0007 (8)	0.0023 (7)
N1	0.0570 (11)	0.0512 (10)	0.0345 (9)	−0.0208 (8)	0.0017 (8)	0.0025 (8)

N4	0.0391 (9)	0.0361 (8)	0.0541 (10)	0.0004 (7)	−0.0125 (8)	−0.0127 (7)
N5	0.0513 (10)	0.0511 (10)	0.0395 (9)	−0.0182 (8)	−0.0043 (8)	−0.0090 (8)
N6	0.0517 (10)	0.0450 (9)	0.0375 (9)	−0.0177 (8)	−0.0080 (8)	−0.0038 (7)
N7	0.0780 (15)	0.0757 (15)	0.0653 (14)	−0.0183 (12)	−0.0273 (12)	−0.0168 (12)
C26	0.0747 (17)	0.0638 (15)	0.0627 (16)	−0.0141 (13)	−0.0104 (13)	−0.0247 (12)
C3	0.0515 (13)	0.0444 (12)	0.0731 (16)	0.0079 (10)	−0.0148 (12)	−0.0148 (11)
C2	0.0566 (13)	0.0598 (13)	0.0332 (11)	−0.0254 (11)	0.0003 (9)	0.0016 (9)
C1	0.0663 (14)	0.0579 (13)	0.0349 (11)	−0.0274 (11)	0.0017 (10)	0.0015 (10)
C4	0.0424 (11)	0.0383 (10)	0.0636 (14)	0.0011 (9)	−0.0189 (10)	−0.0162 (10)
C5	0.0677 (15)	0.0672 (15)	0.0414 (12)	−0.0327 (13)	0.0031 (11)	−0.0089 (11)
C6	0.103 (2)	0.0478 (13)	0.0464 (13)	−0.0329 (14)	−0.0056 (13)	−0.0022 (10)
C7	0.090 (2)	0.0433 (13)	0.0573 (15)	−0.0114 (13)	−0.0043 (14)	−0.0107 (11)
C8	0.0627 (14)	0.0482 (12)	0.0491 (13)	−0.0138 (11)	0.0050 (11)	−0.0087 (10)
C9	0.0516 (12)	0.0421 (10)	0.0383 (11)	−0.0199 (9)	−0.0060 (9)	−0.0105 (8)
C10	0.0500 (12)	0.0423 (11)	0.0462 (11)	−0.0165 (9)	−0.0036 (9)	−0.0108 (9)
C11	0.0642 (14)	0.0580 (13)	0.0425 (12)	−0.0310 (12)	−0.0055 (10)	−0.0008 (10)
C12	0.0448 (12)	0.0818 (17)	0.0503 (13)	−0.0248 (12)	−0.0002 (10)	−0.0073 (12)
C13	0.0452 (12)	0.0687 (16)	0.0562 (14)	−0.0060 (11)	−0.0112 (11)	−0.0042 (12)
C14	0.0489 (12)	0.0544 (12)	0.0428 (12)	−0.0122 (10)	−0.0103 (10)	0.0036 (10)
C15	0.0431 (10)	0.0472 (11)	0.0352 (10)	−0.0190 (9)	−0.0102 (8)	−0.0040 (8)
C16	0.0423 (11)	0.0463 (11)	0.0430 (11)	−0.0141 (9)	−0.0099 (9)	−0.0034 (9)
C17	0.095 (2)	0.084 (2)	0.0752 (19)	−0.0251 (17)	−0.0280 (17)	−0.0129 (16)
C18	0.084 (2)	0.092 (2)	0.096 (2)	−0.0307 (17)	−0.0325 (18)	−0.0203 (19)
C19	0.086 (2)	0.109 (3)	0.092 (2)	−0.0224 (19)	−0.0425 (19)	−0.034 (2)
C20	0.0716 (17)	0.089 (2)	0.0643 (17)	−0.0151 (15)	−0.0242 (14)	−0.0176 (15)
C21	0.0434 (12)	0.0682 (15)	0.0641 (15)	−0.0006 (11)	−0.0167 (11)	−0.0247 (13)
C22	0.0491 (13)	0.0804 (18)	0.0590 (16)	−0.0037 (13)	−0.0168 (12)	−0.0234 (12)
C23	0.094 (2)	0.0747 (19)	0.088 (2)	−0.0216 (17)	−0.0221 (18)	−0.0403 (17)
C24	0.083 (2)	0.0746 (18)	0.090 (2)	−0.0330 (16)	−0.0194 (17)	−0.0229 (16)
C25	0.0807 (19)	0.089 (2)	0.0634 (17)	−0.0311 (16)	−0.0094 (14)	−0.0180 (14)
N8	0.0666 (13)	0.0675 (13)	0.0563 (12)	−0.0171 (11)	−0.0154 (10)	−0.0189 (10)
C27	0.0594 (13)	0.0383 (11)	0.0583 (14)	−0.0029 (10)	−0.0216 (11)	−0.0111 (10)
C28	0.0711 (16)	0.0411 (11)	0.0533 (14)	−0.0038 (11)	−0.0189 (11)	−0.0124 (10)

Geometric parameters (Å, º)

Ag3—C4^{i}	2.0449 (19)	C8—H8	0.9300
Ag3—C3	2.048 (2)	C9—C10	1.465 (3)
Ag2—C2^{ii}	2.056 (2)	C10—C10^{v}	1.326 (4)
Ag2—C2	2.056 (2)	C10—H10	0.9300
Ag1—C1	2.058 (2)	C11—C12	1.364 (3)
Ag1—C1^{iii}	2.058 (2)	C11—H11	0.9300
Fe—O1	2.1365 (15)	C12—C13	1.368 (3)
Fe—O2	2.1392 (16)	C12—H12	0.9300
Fe—N1	2.1440 (17)	C13—C14	1.378 (3)
Fe—N4	2.1489 (16)	C13—H13	0.9300
Fe—N2	2.1522 (16)	C14—C15	1.377 (3)
Fe—N3	2.1539 (17)	C14—H14	0.9300

O1—H1W	0.75 (2)	C15—C16	1.462 (3)
O1—H2W	0.76 (2)	C16—C16^{vi}	1.324 (4)
O2—H3W	0.74 (2)	C16—H16	0.9300
O2—H4W	0.73 (3)	C17—C18	1.360 (4)
N3—C3	1.133 (3)	C17—H17	0.9300
N2—C2	1.129 (3)	C18—C19	1.367 (4)
N1—C1	1.126 (3)	C18—H18	0.9300
N4—C4	1.133 (2)	C19—C20	1.374 (4)
N5—C5	1.333 (3)	C19—H19	0.9300
N5—C9	1.343 (2)	C20—C21	1.386 (3)
N6—C11	1.332 (3)	C20—H20	0.9300
N6—C15	1.347 (2)	C21—C22	1.471 (4)
N7—C17	1.327 (3)	C22—C22^{vii}	1.322 (5)
N7—C21	1.336 (3)	C22—H22	0.9300
C26—C23	1.378 (4)	C23—C24	1.352 (4)
C26—C27	1.387 (3)	C23—H23	0.9300
C26—H26	0.9300	C24—C25	1.371 (3)
C4—Ag3^{iv}	2.0449 (19)	C24—H24	0.9300
C5—C6	1.369 (3)	C25—N8	1.318 (3)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.360 (3)	N8—C27	1.335 (3)
C6—H6	0.9300	C27—C28	1.469 (3)
C7—C8	1.369 (3)	C28—C28^{viii}	1.320 (5)
C7—H7	0.9300	C28—H28	0.9300
C8—C9	1.382 (3)		

C4^{i}—Ag3—C3	179.00 (8)	C10^{v}—C10—H10	117.5
C2^{ii}—Ag2—C2	180.000 (1)	C9—C10—H10	117.5
C1—Ag1—C1^{iii}	180.00 (16)	N6—C11—C12	123.8 (2)
O1—Fe—O2	177.77 (6)	N6—C11—H11	118.1
O1—Fe—N1	88.80 (6)	C12—C11—H11	118.1
O2—Fe—N1	90.70 (7)	C11—C12—C13	118.7 (2)
O1—Fe—N4	88.18 (7)	C11—C12—H12	120.7
O2—Fe—N4	89.65 (7)	C13—C12—H12	120.7
N1—Fe—N4	90.30 (7)	C12—C13—C14	118.5 (2)
O1—Fe—N2	90.90 (6)	C12—C13—H13	120.7
O2—Fe—N2	89.60 (6)	C14—C13—H13	120.7
N1—Fe—N2	179.69 (6)	C15—C14—C13	119.9 (2)
N4—Fe—N2	89.68 (7)	C15—C14—H14	120.0
O1—Fe—N3	91.17 (7)	C13—C14—H14	120.0
O2—Fe—N3	91.00 (7)	N6—C15—C14	121.16 (19)
N1—Fe—N3	89.61 (7)	N6—C15—C16	115.02 (17)
N4—Fe—N3	179.35 (6)	C14—C15—C16	123.81 (18)
N2—Fe—N3	90.41 (7)	C16^{vi}—C16—C15	125.7 (2)
Fe—O1—H1W	126.2 (17)	C16^{vi}—C16—H16	117.2
Fe—O1—H2W	119.1 (19)	C15—C16—H16	117.2
H1W—O1—H2W	106 (2)	N7—C17—C18	124.3 (3)
Fe—O2—H3W	123.3 (19)	N7—C17—H17	117.9

Fe—O2—H4W	116 (2)	C18—C17—H17	117.9
H3W—O2—H4W	106 (3)	C17—C18—C19	117.6 (3)
C3—N3—Fe	178.0 (2)	C17—C18—H18	121.2
C2—N2—Fe	174.23 (18)	C19—C18—H18	121.2
C1—N1—Fe	176.22 (19)	C18—C19—C20	119.7 (3)
C4—N4—Fe	177.91 (19)	C18—C19—H19	120.2
C5—N5—C9	117.53 (19)	C20—C19—H19	120.2
C11—N6—C15	117.80 (18)	C19—C20—C21	119.2 (3)
C17—N7—C21	118.4 (2)	C19—C20—H20	120.4
C23—C26—C27	119.3 (3)	C21—C20—H20	120.4
C23—C26—H26	120.4	N7—C21—C20	120.8 (3)
C27—C26—H26	120.4	N7—C21—C22	114.9 (2)
N3—C3—Ag3	179.1 (2)	C20—C21—C22	124.3 (3)
N2—C2—Ag2	176.6 (2)	$C22^{vii}$—C22—C21	124.8 (3)
N1—C1—Ag1	175.4 (2)	$C22^{vii}$—C22—H22	117.6
N4—C4—$Ag3^{iv}$	178.9 (2)	C21—C22—H22	117.6
N5—C5—C6	124.1 (2)	C24—C23—C26	119.5 (3)
N5—C5—H5	118.0	C24—C23—H23	120.2
C6—C5—H5	118.0	C26—C23—H23	120.2
C7—C6—C5	118.0 (2)	C23—C24—C25	117.7 (3)
C7—C6—H6	121.0	C23—C24—H24	121.1
C5—C6—H6	121.0	C25—C24—H24	121.1
C6—C7—C8	119.4 (2)	N8—C25—C24	124.3 (3)
C6—C7—H7	120.3	N8—C25—H25	117.9
C8—C7—H7	120.3	C24—C25—H25	117.9
C7—C8—C9	119.7 (2)	C25—N8—C27	118.2 (2)
C7—C8—H8	120.2	N8—C27—C26	120.8 (2)
C9—C8—H8	120.2	N8—C27—C28	115.41 (19)
N5—C9—C8	121.18 (19)	C26—C27—C28	123.8 (2)
N5—C9—C10	115.36 (18)	$C28^{viii}$—C28—C27	125.7 (3)
C8—C9—C10	123.46 (19)	$C28^{viii}$—C28—H28	117.2
$C10^{v}$—C10—C9	125.1 (2)	C27—C28—H28	117.2

O1—Fe—N3—C3	−98 (7)	C7—C8—C9—C10	−176.4 (2)
O2—Fe—N3—C3	82 (7)	N5—C9—C10—$C10^{v}$	−158.2 (3)
N1—Fe—N3—C3	−9 (7)	C8—C9—C10—$C10^{v}$	21.1 (4)
N4—Fe—N3—C3	−91 (9)	C15—N6—C11—C12	1.8 (3)
N2—Fe—N3—C3	172 (7)	N6—C11—C12—C13	0.6 (4)
O1—Fe—N2—C2	6.4 (19)	C11—C12—C13—C14	−2.0 (4)
O2—Fe—N2—C2	−171.4 (19)	C12—C13—C14—C15	1.0 (4)
N1—Fe—N2—C2	5 (14)	C11—N6—C15—C14	−2.8 (3)
N4—Fe—N2—C2	−81.7 (19)	C11—N6—C15—C16	176.90 (17)
N3—Fe—N2—C2	97.6 (19)	C13—C14—C15—N6	1.5 (3)
O1—Fe—N1—C1	153 (3)	C13—C14—C15—C16	−178.2 (2)
O2—Fe—N1—C1	−29 (3)	N6—C15—C16—$C16^{vi}$	−159.6 (3)
N4—Fe—N1—C1	−119 (3)	C14—C15—C16—$C16^{vi}$	20.1 (4)
N2—Fe—N1—C1	155 (12)	C21—N7—C17—C18	1.7 (4)
N3—Fe—N1—C1	62 (3)	N7—C17—C18—C19	1.1 (5)

O1—Fe—N4—C4	−34 (5)	C17—C18—C19—C20	−1.9 (5)
O2—Fe—N4—C4	146 (5)	C18—C19—C20—C21	0.0 (5)
N1—Fe—N4—C4	−123 (5)	C17—N7—C21—C20	−3.8 (4)
N2—Fe—N4—C4	57 (5)	C17—N7—C21—C22	176.0 (2)
N3—Fe—N4—C4	−41 (9)	C19—C20—C21—N7	3.0 (4)
Fe—N3—C3—Ag3	−52 (20)	C19—C20—C21—C22	−176.8 (3)
C4^{i}—Ag3—C3—N3	−52 (18)	N7—C21—C22—C22^{vii}	−167.0 (3)
Fe—N2—C2—Ag2	−54 (5)	C20—C21—C22—C22^{vii}	12.9 (5)
C2^{ii}—Ag2—C2—N2	95 (100)	C27—C26—C23—C24	−0.2 (4)
Fe—N1—C1—Ag1	−20 (6)	C26—C23—C24—C25	−2.4 (5)
C1^{iii}—Ag1—C1—N1	−164 (100)	C23—C24—C25—N8	2.5 (5)
Fe—N4—C4—Ag3^{iv}	−78 (13)	C24—C25—N8—C27	0.4 (4)
C9—N5—C5—C6	0.7 (3)	C25—N8—C27—C26	−3.2 (3)
N5—C5—C6—C7	2.2 (4)	C25—N8—C27—C28	175.4 (2)
C5—C6—C7—C8	−2.6 (4)	C23—C26—C27—N8	3.2 (4)
C6—C7—C8—C9	0.2 (4)	C23—C26—C27—C28	−175.4 (2)
C5—N5—C9—C8	−3.3 (3)	N8—C27—C28—C28^{viii}	−167.6 (3)
C5—N5—C9—C10	176.02 (18)	C26—C27—C28—C28^{viii}	11.0 (4)
C7—C8—C9—N5	2.9 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H2*W*···N5	0.76 (3)	2.07 (3)	2.829 (2)	174 (2)
O2—H4*W*···N6	0.73 (3)	2.09 (3)	2.823 (3)	174 (3)
O1—H1*W*···N7^{ix}	0.75 (3)	2.14 (3)	2.870 (3)	164
O2—H3*W*···N8^{x}	0.74 (3)	2.15 (3)	2.868 (3)	162

Symmetry codes: (ix) $x-1, y, z$; (x) $x, y+1, z$.