

Crystal structure of *catena*-poly[[gold(I)- μ -cyanido-[diaquabis(2-phenylpyrazine)iron(II)]- μ -cyanido]dicyanidogold(I)]

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Keywords: crystal structure; polymeric complex; iron(II) complex; 2-phenylpyrazine; dicyanoaurate; aurophillic interactions; offset π - π interactions; supramolecular metal-organic framework.

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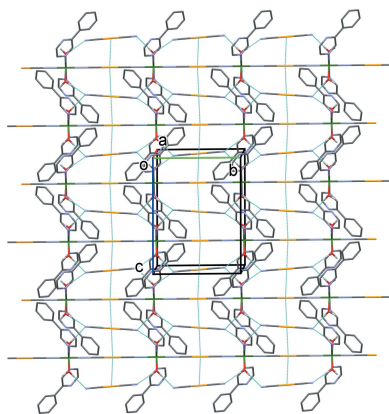
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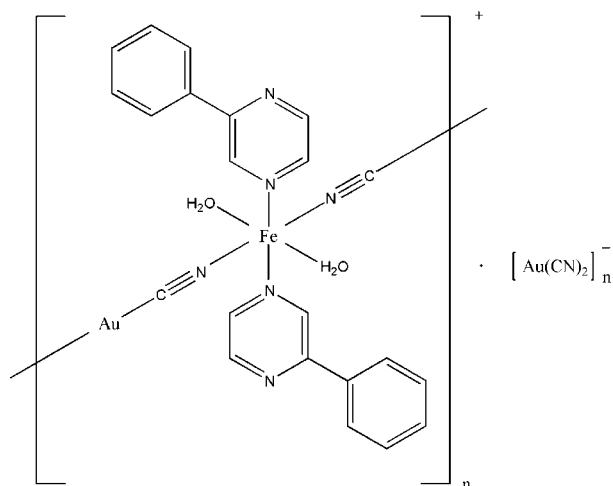
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In the title polymeric complex, $\{[\text{Fe}(\text{CN})_2(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2][\text{Au}(\text{CN})_2]\}_n$, the Fe^{II} ion, which is located on a twofold rotation axis, has a slightly distorted FeN_4O_2 octahedral geometry. It is coordinated by two phenylpyrazine molecules, two water molecules and two dicyanoaurate anions, the Au atom also being located on a second twofold rotation axis. In the crystal, the coordinated dicyanoaurate anions bridge the Fe^{II} ions to form polymeric chains propagating along the *b*-axis direction. In the crystal, the chains are linked by $\text{O}_{\text{water}}-\text{H}\cdots\text{N}_{\text{dicyanoaurate}}$ hydrogen bonds and aurophillic interactions [$\text{Au}\cdots\text{Au} = 3.5661(3) \text{ \AA}$], forming layers parallel to the *bc* plane. The layers are linked by offset π - π stacking interactions [intercentroid distance = $3.643(3) \text{ \AA}$], forming a supramolecular metal-organic framework.

1. Chemical context

The design of functional materials based on coordination compounds is an important area of current scientific research. For example, metal-organic frameworks (MOFs), which consist of metal ions and organic ligand linkers, are studied intensively. Fe-based coordination polymers with N-donor bridging ligands are well known as compounds with switchable spin states (Niel *et al.*, 2003; Gural'skiy *et al.*, 2016; Kucheriv *et al.*, 2016). This phenomenon is called spin crossover and can be observed in complexes of $3d^4$ - $3d^7$ metal ions. Applying external stimuli, such as temperature, pressure, magnetic field, light irradiation or adding a guest can affect this kind of the compound and change their properties significantly (Gütlich & Goodwin, 2004). The synthesis and crystallographic characterization of these complexes are of current interest because of the bistability of their magnetic, electrical, mechanical and optical properties (Senthil Kumar & Ruben, 2017). The parameters of these transitions could be controlled through a wide variety of available organic ligands and co-ligands. Complexes with metallocyanate bridges as co-ligands to N-bridging ligands form one of the largest family of spin-crossover compounds (Muñoz & Real, 2011). Here we report on a new one-dimensional polymeric compound that is similar in its structure to switchable cyanometallates. It employs 2-phenylpyrazine as a ligand and $\text{Au}(\text{CN})_2^{2-}$ as co-ligands, while coordinated H_2O molecules stabilize the Fe^{II} ions in the high-spin state.





2. Structural commentary

The structure of the title compound features a one-dimensional chain motif that runs parallel to the crystallographic *b* axis (Figs. 1 and 2). The compound crystallizes in the monoclinic space group *C2/c*. Selected bond distances and bond angles are given in Table 1. The coordination sphere of the Fe^{II} cation, atom Fe1, which is located on a twofold rotation axis, has a distorted octahedral environment [FeN₄O₂]. It includes two 2-phenylpyrazine N atoms [Fe1–N3 = 2.223 (5) Å] in axial positions, and two N atoms of cyano bridges and two water O atoms of water molecules [Fe1–O1 = 2.122 (4) Å] in equatorial positions. The two CN[−] anions bridge the Fe^{II} and Au^I cations [Fe1···Au1 = 5.244 (3) Å] to form a one-dimensional polymeric structure with bond lengths Fe1–N1 = 2.107 (5) Å and Fe1–N2 = 2.117 (6) Å (Fig. 1 and Table 1).

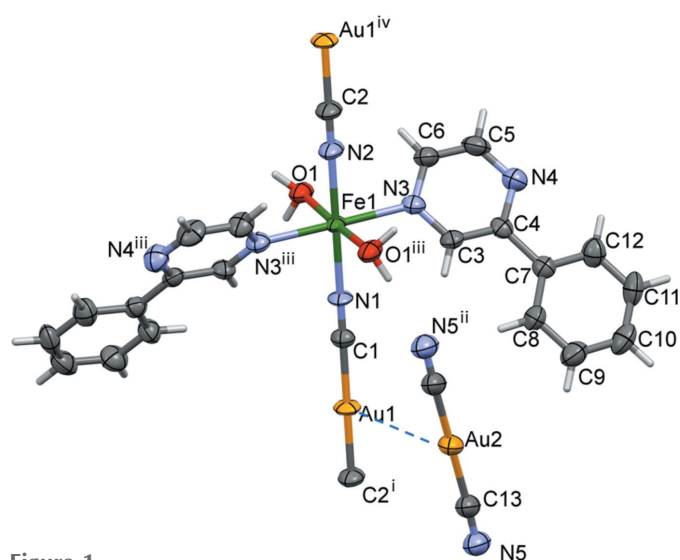


Figure 1

A fragment of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The Au1···Au2 interaction [3.5661 (3) Å] is shown as a dashed line. [Symmetry codes: (i) $x, y - 1, z$; (ii) $x - 1, y - 1, z - 1$; (iii) $-x - 1, y, -z + \frac{3}{2}$; (iv) $x, y + 1, z$].

Table 1

Selected geometric parameters (Å, °).

Au1–C1	1.975 (7)	Fe1–N2	2.117 (6)
Au1–C2 ⁱ	1.988 (7)	Fe1–O1	2.122 (4)
Au2–C13	1.988 (6)	Fe1–N3	2.223 (5)
Fe1–N1	2.107 (5)		
C1–Au1–C2 ⁱ	180	N2–Fe1–N3	89.60 (10)
C13 ⁱⁱⁱ –Au2–C13	180	O1–Fe1–N3	90.09 (16)
N1–Fe1–N2	180	C1–N1–Fe1	180
O1–Fe1–O1 ⁱⁱⁱ	176.73 (19)	C2–N2–Fe1	180
N3–Fe1–N3 ⁱⁱⁱ	179.19 (19)	N1–C1–Au1	180
N1–Fe1–O1	91.63 (9)	N2–C2–Au1 ^{iv}	180
N2–Fe1–O1	88.37 (9)	N5–C13–Au2	175.8 (7)
N1–Fe1–N3	90.40 (10)		

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

The Fe^{II} octahedral distortion parameter (the sum of the moduli of the deviations from 90° for all *cis*-bond angles) is $\Sigma|90 - \Theta| = 8.53^\circ$, where Θ are the *cis*-N–Fe–O and *cis*-N–Fe–N angles in the coordination environment of the Fe^{II} atom.

3. Supramolecular features

The crystal packing features different types of weak interactions (see Table 2 and Figs. 2 and 3). The free dicyanoaurate anions are linked to the polymeric chains by O_{water}–H···N hydrogen bonds [O1–H1A···N5^v = 2.02 Å and O1–H1B···N5^{vi} = 2.18 Å; Table 2], and by aurophilic interactions [Au1···Au2 = 3.566 (2) Å], forming layers parallel to the *bc*

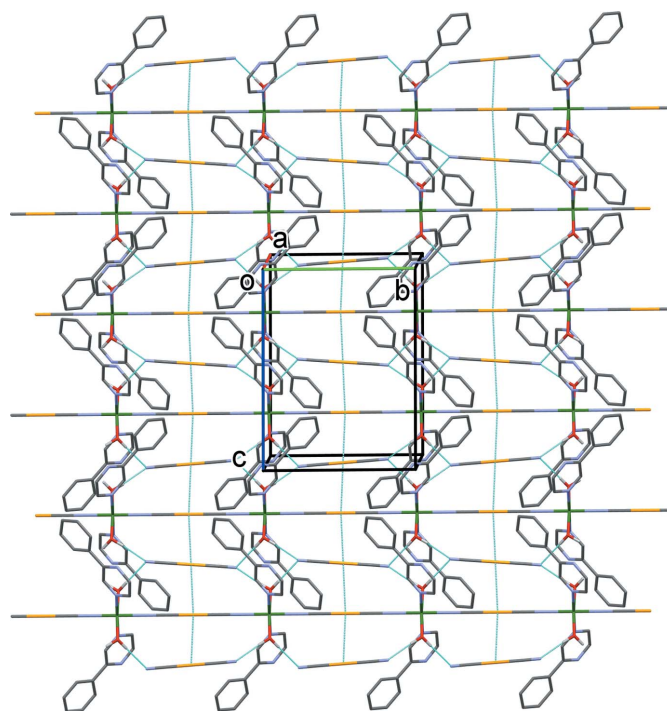


Figure 2

A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds (Table 2) and aurophilic interactions as shown as dashed lines. For clarity, the C-bound H atoms have been omitted.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1A\cdots N5^v$	0.86	2.02	2.851 (6)	165
$O1-H1B\cdots N5^{vi}$	0.85	2.18	3.023 (6)	178

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

plane. The layers are then linked *via* offset π - π interactions involving a pyrazine ring as an acceptor and a phenyl ring as a donor of electron density, forming a supramolecular metal-organic framework [$Cg1\cdots Cg2 = 3.643$ (3) Å, where $Cg1$ and $Cg2$ are the centroids of the $N3/N4/C3-C6$ and $C7-C12$ rings, respectively; $\alpha = 3.8$ (3)°, interplanar distances = 3.466 (2) and 3.510 (2) Å, offset = 0.976 Å, symmetry code (i): $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$].

4. Database survey

A survey of the Cambridge Structural Database (Version 5.38; Groom *et al.*, 2016) confirmed that the structure of the title complex has not been reported previously and revealed 41 Fe-Au CN-bridged frameworks supported axially by different co-ligands. There are 37 compounds with an octahedral FeN_6 environment. The coordination spheres of such compounds are formed by pyridine-azine ligands, substituted pyridines, saturated and substituted pyrazines, and pyrimidine (Clements *et al.*, 2016; Arcís-Castillo *et al.*, 2013; Agustí *et al.*, 2008; Clements *et al.*, 2014, Kosone & Kitazawa, 2016; Niel *et al.*, 2003). Nine such compounds have a stable low- or high-spin state and another 28 are complexes with a switchable spin state. There are also four compounds with an environment formed by the N atoms of organic ligands and water O atoms. The only compound with an FeN_5O environment contains a pyridine-based N-donor ligand (Xu *et al.*, 2014), while three compounds have an FeN_4O_2 octahedral geometry. The bidentate bridging organoselenium triazole ligand and two different pyridine-based ligands were used to obtain these latter complexes (Seredyuk *et al.*, 2007; Xu *et al.*, 2014).

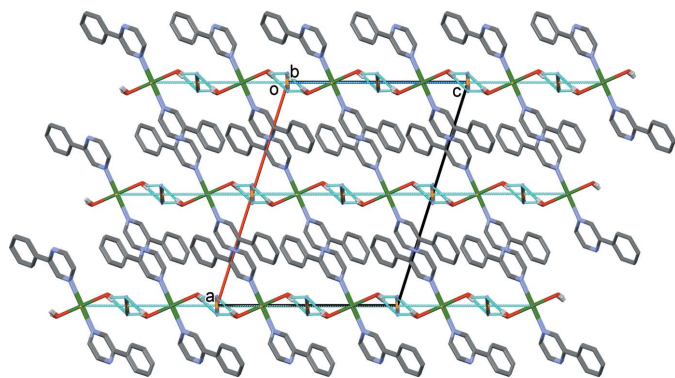


Figure 3
A view along the b axis of the crystal packing of the title compound. The $O-H\cdots N$ hydrogen bonds and $Au\cdots Au$ interactions are shown as dashed lines. For clarity, the C-bound H atoms have been omitted.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[AuFe(CN)_2(C_{10}H_8N_2)_2(H_2O)_2]\cdot [Au(CN)_2]$
M_r	902.26
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	293
a, b, c (Å)	18.5306 (13), 10.4541 (3), 14.2522 (9)
β (°)	107.509 (7)
V (Å ³)	2633.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	11.70
Crystal size (mm)	$0.3 \times 0.3 \times 0.1$
Data collection	
Diffractometer	Rigaku Xcalibur Eos
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2015)
T_{min}, T_{max}	0.292, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7203, 3265, 2410
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.038, 0.084, 1.04
No. of reflections	3265
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	1.37, -1.45

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELX2018* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

5. Synthesis and crystallization

Crystals of the title compound were prepared by the slow diffusion method between three layers in a 10 ml tube. The first layer was a solution of $K[Au(CN)_2]$ (0.0058 g, 0.02 mmol) in water (2.5 ml), the second was a mixture of water/acetonitrile (1:2, 5 ml) and the third layer was a solution of 2-phenylpyrazine (0.0078 g, 0.05 mmol) and $[Fe(OTs)_2]\cdot 6H_2O$ (0.0101 g, 0.02 mmol) (OTs = *p*-toluenesulfonate) in acetonitrile (2.5 ml) with 0.3 ml of water. After two weeks, yellow crystals grew in the second layer; these were collected and maintained under the mother solution until measured.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were placed in their expected calculated positions ($C-H = 0.93$ Å) and refined as riding with $U_{iso}(H) = 1.2U_{iso}(C)$. The idealized OH_2 group was fixed using an AFIX 7 command that allowed the H atoms to ride on the O atom and rotate around the bond.

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supporting information

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

catena-Poly[[gold(I)- μ -cyanido-[diaquabis(2-phenylpyrazine)iron(II)]- μ -cyanido] dicyanidogold(I)]

Crystal data

[AuFe(CN)₂(C₁₀H₈N₂)₂(H₂O)₂][Au(CN)₂]
 $M_r = 902.26$
 Monoclinic, *C2/c*
 $a = 18.5306$ (13) Å
 $b = 10.4541$ (3) Å
 $c = 14.2522$ (9) Å
 $\beta = 107.509$ (7)°
 $V = 2633.0$ (3) Å³
 $Z = 4$

$F(000) = 1680$
 $D_x = 2.276$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 2258 reflections
 $\theta = 2.3$ – 30.8 °
 $\mu = 11.70$ mm⁻¹
 $T = 293$ K
 Plate, clear light yellow
 $0.3 \times 0.3 \times 0.1$ mm

Data collection

Rigaku Xcalibur Eos
 diffractometer
 Radiation source: fine-focus sealed X-ray tube,
 Enhance (Mo) X-ray Source
 Graphite monochromator
 Detector resolution: 8.0797 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (CrysAlis PRO; Rigaku OD, 2015)

$T_{\min} = 0.292$, $T_{\max} = 1.000$
 7203 measured reflections
 3265 independent reflections
 2410 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 28.3$ °, $\theta_{\min} = 2.3$ °
 $h = -17 \rightarrow 24$
 $k = -7 \rightarrow 13$
 $l = -18 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.084$
 $S = 1.04$
 3265 reflections
 173 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map
 Hydrogen site location: mixed
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.2566P]$
 where $P = (F_o^2 + 2F_c^2)/3$

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

$$\Delta\rho_{\max} = 1.37 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.45 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.500000	0.51420 (2)	0.750000	0.03916 (11)
Au2	0.500000	0.500000	0.500000	0.04886 (13)
Fe1	0.500000	1.01389 (8)	0.750000	0.0304 (3)
O1	0.4511 (3)	1.0197 (3)	0.8669 (2)	0.0440 (10)
H1A	0.461953	0.949471	0.898996	0.066*
H1B	0.474896	1.072647	0.910236	0.066*
C12	0.2099 (3)	0.8548 (6)	0.3359 (4)	0.0498 (16)
H12	0.177175	0.921680	0.337514	0.060*
N3	0.3852 (3)	1.0154 (3)	0.6414 (3)	0.0372 (11)
N1	0.500000	0.8124 (5)	0.750000	0.0381 (16)
C1	0.500000	0.7031 (6)	0.750000	0.0347 (18)
N4	0.2472 (3)	1.0277 (4)	0.4918 (3)	0.0487 (13)
C3	0.3652 (3)	0.9310 (4)	0.5669 (4)	0.0366 (13)
H3	0.398880	0.865572	0.565374	0.044*
C9	0.3032 (4)	0.6538 (5)	0.3300 (4)	0.0556 (17)
H9	0.335120	0.585689	0.328588	0.067*
C13	0.4723 (4)	0.3157 (6)	0.4880 (4)	0.0519 (17)
C7	0.2772 (3)	0.8418 (5)	0.4104 (4)	0.0355 (12)
C6	0.3334 (3)	1.1041 (5)	0.6411 (4)	0.0453 (15)
H6	0.343207	1.163949	0.691614	0.054*
N5	0.4606 (3)	0.2077 (5)	0.4804 (3)	0.0572 (15)
N2	0.500000	1.2164 (5)	0.750000	0.0465 (19)
C10	0.2365 (4)	0.6684 (6)	0.2558 (4)	0.0558 (18)
H10	0.222790	0.609994	0.204193	0.067*
C8	0.3230 (3)	0.7399 (5)	0.4067 (4)	0.0448 (15)
H8	0.368242	0.728887	0.456743	0.054*
C5	0.2662 (4)	1.1083 (5)	0.5674 (4)	0.0518 (16)
H5	0.231568	1.171427	0.570352	0.062*
C11	0.1910 (4)	0.7682 (6)	0.2584 (4)	0.0553 (17)
H11	0.146242	0.779119	0.207499	0.066*
C4	0.2977 (3)	0.9364 (4)	0.4927 (4)	0.0336 (12)
C2	0.500000	1.3240 (7)	0.750000	0.045 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0509 (2)	0.01133 (13)	0.0543 (2)	0.000	0.01452 (16)	0.000

Au2	0.0638 (3)	0.02992 (17)	0.0467 (2)	0.00972 (13)	0.00732 (17)	-0.00062 (12)
Fe1	0.0484 (7)	0.0125 (4)	0.0289 (5)	0.000	0.0094 (5)	0.000
O1	0.069 (3)	0.0265 (17)	0.035 (2)	0.0036 (17)	0.0132 (19)	-0.0003 (15)
C12	0.041 (4)	0.062 (4)	0.045 (4)	-0.003 (3)	0.011 (3)	-0.002 (3)
N3	0.045 (3)	0.025 (2)	0.041 (3)	0.0041 (18)	0.011 (2)	0.0012 (18)
N1	0.055 (5)	0.010 (2)	0.045 (4)	0.000	0.010 (3)	0.000
C1	0.038 (5)	0.026 (4)	0.041 (4)	0.000	0.013 (3)	0.000
N4	0.052 (3)	0.044 (2)	0.047 (3)	0.012 (2)	0.011 (2)	0.001 (2)
C3	0.043 (4)	0.023 (2)	0.042 (3)	-0.001 (2)	0.010 (3)	-0.003 (2)
C9	0.070 (5)	0.045 (3)	0.051 (4)	-0.004 (3)	0.018 (3)	-0.010 (3)
C13	0.071 (5)	0.041 (3)	0.040 (3)	0.012 (3)	0.011 (3)	-0.001 (3)
C7	0.036 (3)	0.034 (3)	0.037 (3)	-0.002 (2)	0.013 (2)	0.003 (2)
C6	0.058 (4)	0.034 (3)	0.044 (3)	0.011 (3)	0.015 (3)	-0.003 (2)
N5	0.083 (4)	0.040 (3)	0.047 (3)	0.006 (3)	0.017 (3)	-0.002 (2)
N2	0.075 (6)	0.018 (3)	0.041 (4)	0.000	0.010 (4)	0.000
C10	0.065 (5)	0.055 (4)	0.047 (4)	-0.023 (3)	0.016 (3)	-0.015 (3)
C8	0.045 (4)	0.043 (3)	0.041 (3)	-0.004 (2)	0.005 (3)	-0.008 (2)
C5	0.060 (4)	0.037 (3)	0.060 (4)	0.019 (3)	0.021 (3)	0.004 (3)
C11	0.042 (4)	0.079 (5)	0.037 (4)	-0.016 (3)	0.001 (3)	-0.006 (3)
C4	0.037 (3)	0.029 (2)	0.036 (3)	0.000 (2)	0.012 (2)	0.008 (2)
C2	0.067 (6)	0.019 (3)	0.046 (5)	0.000	0.014 (4)	0.000

Geometric parameters (Å, °)

Au1—C1	1.975 (7)	N4—C5	1.329 (7)
Au1—C2 ⁱ	1.988 (7)	N4—C4	1.333 (7)
Au2—C13 ⁱⁱ	1.988 (6)	C3—C4	1.376 (7)
Au2—C13	1.988 (6)	C3—H3	0.9300
Fe1—N1	2.107 (5)	C9—C10	1.373 (7)
Fe1—N2	2.117 (6)	C9—C8	1.377 (7)
Fe1—O1	2.122 (4)	C9—H9	0.9300
Fe1—O1 ⁱⁱⁱ	2.122 (4)	C13—N5	1.149 (7)
Fe1—N3	2.223 (5)	C7—C8	1.374 (7)
Fe1—N3 ⁱⁱⁱ	2.223 (5)	C7—C4	1.492 (7)
O1—H1A	0.8564	C6—C5	1.368 (7)
O1—H1B	0.8479	C6—H6	0.9300
C12—C7	1.380 (6)	N2—C2	1.125 (8)
C12—C11	1.390 (7)	C10—C11	1.349 (8)
C12—H12	0.9300	C10—H10	0.9300
N3—C6	1.333 (6)	C8—H8	0.9300
N3—C3	1.344 (6)	C5—H5	0.9300
N1—C1	1.143 (8)	C11—H11	0.9300
C1—Au1—C2 ⁱ	180	N3—C3—C4	123.4 (5)
C13 ⁱⁱ —Au2—C13	180	N3—C3—H3	118.3
N1—Fe1—N2	180	C4—C3—H3	118.3
O1—Fe1—O1 ⁱⁱⁱ	176.73 (19)	C10—C9—C8	120.2 (6)
N3—Fe1—N3 ⁱⁱⁱ	179.19 (19)	C10—C9—H9	119.9

N1—Fe1—O1	91.63 (9)	C8—C9—H9	119.9
N2—Fe1—O1	88.37 (9)	N2—C2—Au1 ^{iv}	180
N1—Fe1—O1 ⁱⁱⁱ	91.63 (9)	N5—C13—Au2	175.8 (7)
N2—Fe1—O1 ⁱⁱⁱ	88.37 (9)	C8—C7—C12	118.2 (5)
N1—Fe1—N3	90.40 (10)	C8—C7—C4	122.0 (5)
N2—Fe1—N3	89.60 (10)	C12—C7—C4	119.8 (5)
O1—Fe1—N3	90.09 (16)	N3—C6—C5	120.9 (5)
O1 ⁱⁱⁱ —Fe1—N3	89.89 (16)	N3—C6—H6	119.6
N1—Fe1—N3 ⁱⁱⁱ	90.40 (10)	C5—C6—H6	119.6
N2—Fe1—N3 ⁱⁱⁱ	89.60 (10)	C11—C10—C9	119.3 (6)
O1—Fe1—N3 ⁱⁱⁱ	89.89 (16)	C11—C10—H10	120.3
O1 ⁱⁱⁱ —Fe1—N3 ⁱⁱⁱ	90.09 (16)	C9—C10—H10	120.3
Fe1—O1—H1A	108.0	C7—C8—C9	121.2 (5)
Fe1—O1—H1B	109.9	C7—C8—H8	119.4
H1A—O1—H1B	100.6	C9—C8—H8	119.4
C7—C12—C11	120.1 (6)	N4—C5—C6	124.0 (5)
C7—C12—H12	120.0	N4—C5—H5	118.0
C11—C12—H12	120.0	C6—C5—H5	118.0
C6—N3—C3	115.3 (5)	C10—C11—C12	121.1 (6)
C6—N3—Fe1	123.0 (4)	C10—C11—H11	119.5
C3—N3—Fe1	121.6 (4)	C12—C11—H11	119.5
C1—N1—Fe1	180	N4—C4—C3	120.7 (5)
C2—N2—Fe1	180	N4—C4—C7	117.1 (5)
N1—C1—Au1	180	C3—C4—C7	122.3 (5)
C5—N4—C4	115.6 (5)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots N5 ^v	0.86	2.02	2.851 (6)	165
O1—H1B \cdots N5 ^{vi}	0.85	2.18	3.023 (6)	178

Symmetry codes: (v) $x, -y+1, z+1/2$; (vi) $-x+1, y+1, -z+3/2$.