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Crystal structure of poly[tetra- μ -cyanido-ethanol-bis(2-iodopyrazine)digold(I)iron(II)]

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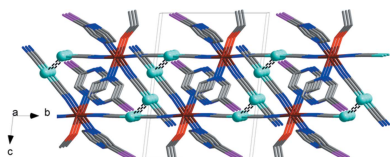
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In the title polymeric complex, $[\text{Au}_2\text{Fe}(\text{CN})_4(\text{C}_4\text{H}_3\text{IN}_2)_2(\text{C}_2\text{H}_6\text{O})]_n$, the Fe^{II} cation is coordinated by two iodopyrazine molecules, one ethanol molecule and three dicyanoaurate anions in a distorted N_5O octahedral geometry. In the crystal, the dicyanoaurate anions bridge the Fe^{II} cations to form polymeric chains propagating along the b -axis direction. Stabilization of the crystal structure is provided by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds and $\pi-\pi$ stacking between parallel iodopyrazine rings of neighbouring chains, the centroid-centroid distances being 3.654 (10) and 3.658 (9) Å.

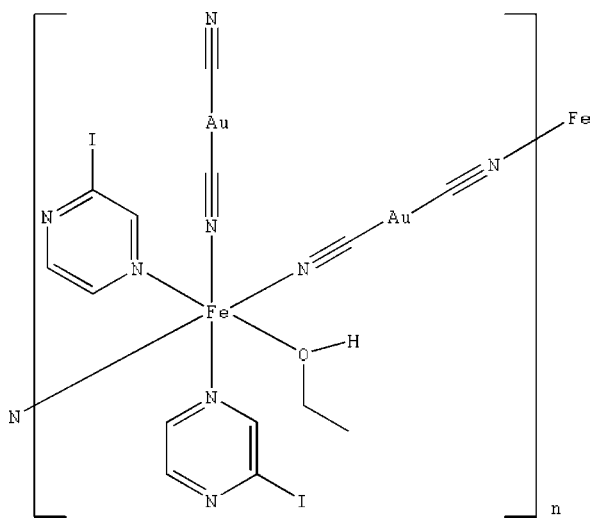
1. Chemical context

Among all coordination compounds, cyanide-based complexes attract considerable attention. The cyanide group can be coordinated in either a monodentate or bridging way, connecting different metal ions, leading to the formation of one-, two- or three-dimensional frameworks. The variety of possible structures of cyanide-based complexes results in a variety of functional properties for these coordination materials, such as the ability to include small guest molecules (Klausmeyer *et al.*, 1998), act as room-temperature magnets (Garde *et al.*, 2002), display photomagnetic and magneto-optical properties (Mizuno *et al.*, 2000; Mercuriol *et al.*, 2010), *etc.* The most representative examples of cyanide-bridged complexes are Prussian blue analogues, which form three-dimensional frameworks with general formula $A^1M_A^{\text{II}}[M_B^{\text{III}}(\text{CN})_6]$ (A = alkali ion, M_A and M_B = transition metal ions; Keggin & Miles, 1936). Prussian blue analogues are very attractive because of their facile synthesis and the possibility to manipulate the magnetic ordering of the material by selecting appropriate spin sources (Ohkoshi *et al.*, 1997).

Cyanometallate complexes are typically characterized by a low-spin state of the metal ions; however, the introduction of a complementary ligand with weak ligand field strength can lead to the formation of spin-crossover compounds. This type of compound is mostly represented by Hofmann clathrate analogues with general formula $[M(L)_x\{M'(\text{CN})_4\}]$ where $M = \text{Fe}^{2+}$, Co^{2+} , Ni^{2+} , Cu^{2+} , Zn^{2+} , Cd^{2+} and Mn^{2+} , $M' = \text{Ni}^{2+}$, Pd^{2+} , Pt^{2+} and L is either a unidentate or bridging ligand. The first compound of this type reported by Hofmann & Höchtlen (1903) was the $[\text{Ni}(\text{NH}_3)_2\{\text{Ni}(\text{CN})_4\}]$ clathrate, which is able to incorporate benzene or other aromatic molecules. In this structure, the bridging tetracyanonikellate anions contribute to the formation of infinite layers that propagate in the ab plane



(Powell & Rayner, 1949). However, the first Hofmann-clathrate analogue displaying spin-crossover behavior was [Fe(py)₂{Ni(CN)₄}] (Kitazawa *et al.*, 1996). Later, different examples have been obtained for the modification of the original Hofmann clathrates, notably with di- or octacyano-metallates (Gural'skiy *et al.*, 2016*b*; Wei *et al.*, 2016). Another modification method is the use of different organic ligands; for example, the inclusion of a bidentate ligand such as pyrazine leads to the formation of a three-dimensional network (Niel *et al.*, 2001). Here we report a new cyanide-based compound with general formula [Fe(Ipz)₂(EtOH){Au(CN)₂}₂] in which the Fe^{II} ions are stabilized in the high-spin state.



2. Structural commentary

The crystal structure of the title compound was determined at 296 K. It crystallizes in the triclinic $P\bar{1}$ space group with two formula units per cell. The Fe^{II} site has a distorted octahedral [FeN₅O] coordination environment formed by two iodo-

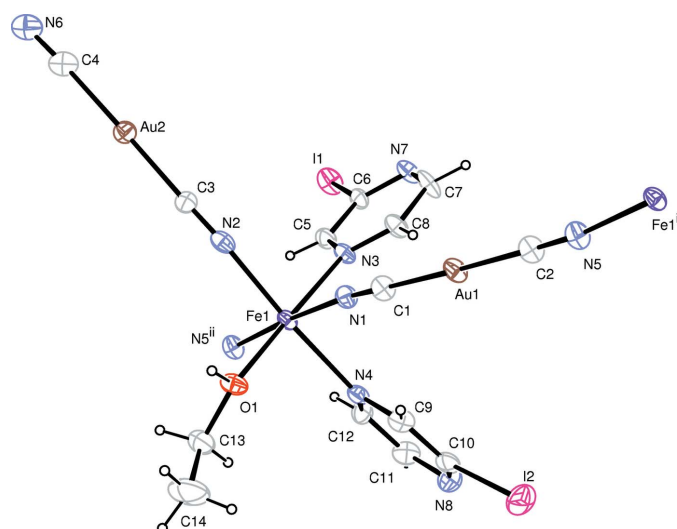


Figure 1
A fragment of the molecular structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) $x, 1 + y, z$; (ii) $x, -1 + y, z$].

Table 1
Selected bond lengths (Å).

Au1—C1	1.948 (9)	Fe1—N1	2.105 (8)
Au1—C2	1.952 (8)	Fe1—N2	2.096 (7)
Au2—C3	1.970 (8)	Fe1—N3	2.272 (7)
Au2—C4	1.981 (9)	Fe1—N4	2.216 (7)
Fe1—O1	2.106 (6)	Fe1—N5 ⁱ	2.096 (8)

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

Table 2
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—H1...N6 ⁱⁱ	0.86 (5)	1.98 (5)	2.765 (13)	151 (6)

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

pyrazine N atoms, three dicyanoaurate N atoms and one ethanol O atom (Fig. 1). Two iodopyrazine molecules are coordinated in the *cis* configuration with the Fe—N distances of 2.216 (7) and 2.272 (7) Å (Table 1) indicating the high-spin state of the Fe^{II} cation. One of the dicyanoaurate fragments is N-coordinated to the Fe^{II} site in the form of an anion [Fe1—N2 = 2.096 (7) Å], while the other two are coordinated in a *trans* configuration, further connecting the framework into a chain [Fe1—N1 = 2.105 (8) and Fe1—N5 = 2.096 (8) Å]. The CN[−] anions bridge the Fe^{II} and Au^I cations in a quasi-linear mode with C1—Au1—C2 = 178.8 (3) and C3—Au2—C4 = 178.9 (3)°. In addition, one of the coordination sites of the Fe^{II} ion is occupied by an O-coordinated ethanol molecule with Fe1—O1 = 2.106 (6) Å, which is a typical value for Fe—O_{alcohol} bonds. There is a deviation from an ideal octahedral geometry, $|\Sigma|90^\circ - \Theta| = 33.1^\circ$, where Θ is the *cis*-N—Fe—N or *cis*-O—Fe—N angle in the coordination environment of Fe^{II}. This value indicates a significant polyhedral distortion that can be explained by the Jahn–Teller effect and the presence of four different types of ligands.

3. Supramolecular features

The coordination framework is connected by bridging dicyanoaurate moieties into chains that propagate along the *b*-axis direction. In addition, the crystal packing is supported by N...H—O hydrogen bonds (Fig. 2*a*, Table 2) in which H atoms from the ethanol hydroxyl group participate in weak interactions with the N atoms of the dicyanoaurate anions. The structure includes parallel-displaced π — π interactions with a distance of 3.381 (5) Å between the planes of the aromatic rings (Fig. 2*b*). Short Au...Au distances of 3.163 (5) Å indicate intermolecular aurophilic interactions between the Au atoms of the monodentate and bridging dicyanoaurate moieties (Fig. 2*c*). The same type of aurophilic interaction was observed for a very similar Au—Fe—pyrazine complex, which displays high-temperature spin-transition behavior [Au...Au (LS, 340 K) = 3.3886 (3) Å, Au...Au (HS, 360 K) = 3.5870 (5) Å; Gural'skiy *et al.*, 2016*a*]. The Au...Au distances in the above-mentioned structure are longer because they are defined by a three-dimensional framework of the complex; however, in the case of the title compound, the dicyanoaurate

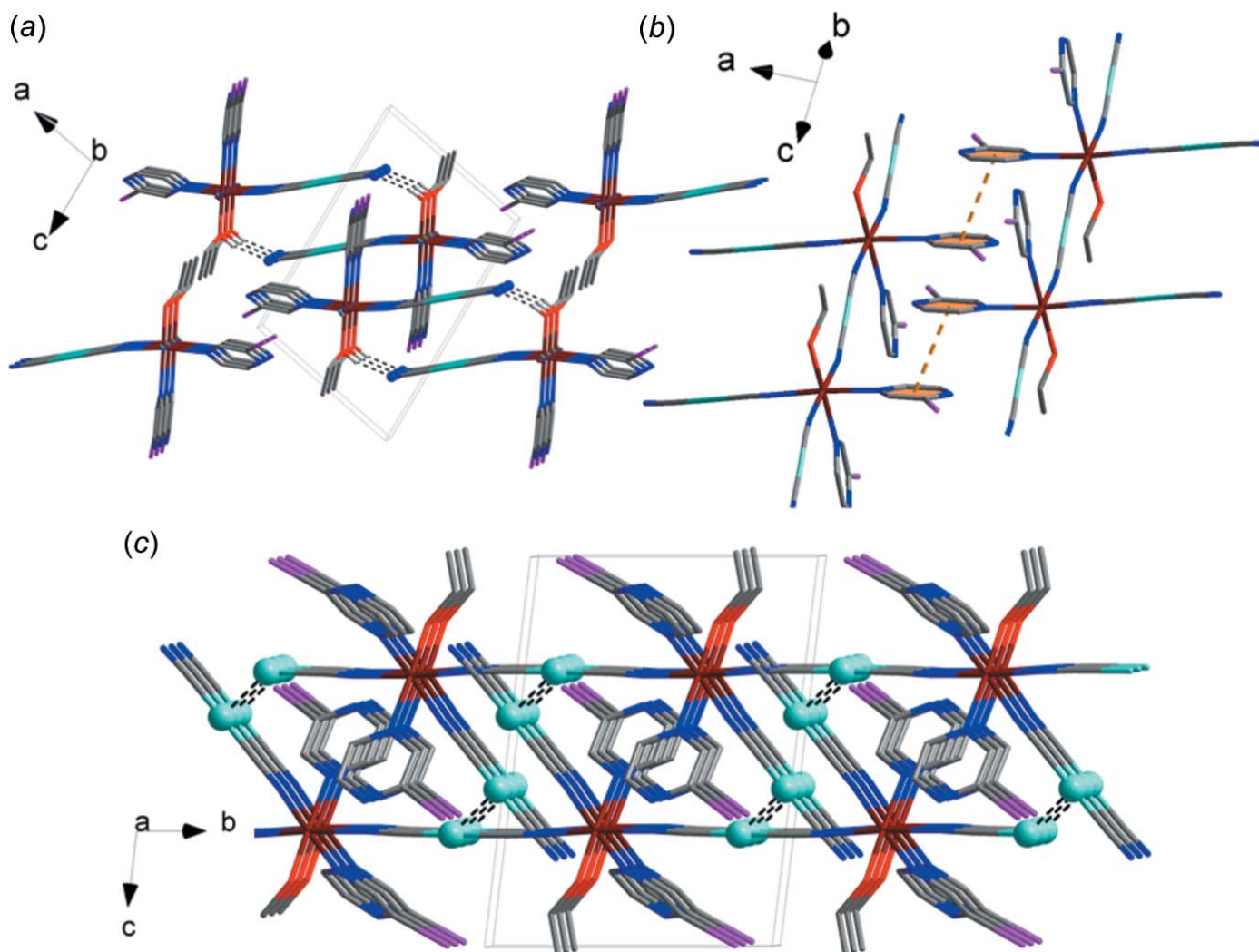


Figure 2

The crystal structure of the title compound. (a) View in the *ac* plane showing N...H—O hydrogen bonds (dashed lines). H atoms, except those involved in hydrogen bonding, are omitted for clarity. (b) Structure of the title compound showing π – π contacts (dashed lines). (c) View in the *bc* plane showing auriphilic interactions (dashed lines). Colour key: Fe dark red; Ag cyan; N blue; O red; C grey; I purple.

anions are non-bridging and therefore are more flexible, which leads to the creation of auriphilic contacts that are closer to the optimum distance of 3 Å (Schmidbaur, 2000).

4. Database survey

A survey of the Cambridge structural Database (Version 5.38; Groom *et al.*, 2016) confirmed that the title compound has never been published before. It also revealed numerous examples of CN-bridged Au–Fe bimetallic frameworks supported by substituted azines (Li *et al.*, 2015; Agustí *et al.*, 2008; Kosone *et al.*, 2009) and non-substituted azines (Niel *et al.*, 2003; Gural'skiy *et al.*, 2016a; Kosone *et al.*, 2008).

5. Synthesis and crystallization

Crystals of the title compound were obtained by the slow-diffusion method with three layers in a 5 ml tube. The first layer was a solution of K[Au(CN)₂] (29 mg, 0.1 mmol) in water

(1 ml), the second layer was a water/ethanol mixture (1:1, 2.5 ml) and the third layer was a solution of Fe(OTs)₂·6H₂O (OTs = toluenesulfonate) (50.6 mg, 0.1 mmol) and iodo-pyrazine (41.2 mg, 0.2 mmol) in ethanol (1 ml). After two weeks, yellow crystals grew in the middle layer; these were collected and kept under the mother solution prior to measurement.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms were placed geometrically at their expected calculated positions with C—H = 0.96 (CH₃), 0.97 (CH₂), 0.93 Å (C_{arom}), O—H = 0.859 (10) Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ with the exception of methyl hydrogen atoms, which were refined with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. The idealized CH₃ group was fixed using an AFIX 137 command that allowed the H atoms to ride on the C atom and rotate around the C—C bond.

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Table 3

Experimental details.

Crystal data	
Chemical formula	[Au ₂ Fe(CN) ₄ (C ₄ H ₃ IN ₂) ₂ (C ₂ H ₆ O)]
<i>M_r</i>	1011.90
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.40 (2), 10.30 (2), 12.81 (3)
α , β , γ (°)	92.05 (6), 99.67 (7), 114.30 (6)
<i>V</i> (Å ³)	1106 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	16.70
Crystal size (mm)	0.20 × 0.05 × 0.03
Data collection	
Diffractometer	Bruker SMART
Absorption correction	Part of the refinement model (ΔF) (Walker & Stuart, 1983)
<i>T</i> _{min} , <i>T</i> _{max}	0.298, 0.456
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	5556, 5556, 4453
<i>R</i> _{int}	0.097
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.680
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.077, 0.92
No. of reflections	5556
No. of parameters	257
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	2.26, -2.28

Computer programs: *SMART* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *DIAMOND* (Brandenburg *et al.*, 1999) and *OLEX2* (Dolomanov *et al.*, 2009).

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Crystal structure of poly[tetra- μ -cyanido-ethanolbis(2-iodopyrazine)-digold(I)iron(II)]

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Computing details

Data collection: *SMART* (Bruker, 2013); cell refinement: *SAINTE* (Bruker, 2013); data reduction: *SAINTE* (Bruker, 2013); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg *et al.*, 1999); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Poly[tetra- μ -cyanido-ethanolbis(2-iodopyrazine)digold(I)iron(II)]

Crystal data

[Au₂Fe(CN)₄(C₄H₃IN₂)₂(C₂H₆O)]

$M_r = 1011.90$

Triclinic, $P\bar{1}$

$a = 9.40$ (2) Å

$b = 10.30$ (2) Å

$c = 12.81$ (3) Å

$\alpha = 92.05$ (6)°

$\beta = 99.67$ (7)°

$\gamma = 114.30$ (6)°

$V = 1106$ (4) Å³

$Z = 2$

$F(000) = 900$

$D_x = 3.039$ Mg m⁻³

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

Cell parameters from 5517 reflections

$\theta = 2.4$ – 28.1 °

$\mu = 16.70$ mm⁻¹

$T = 296$ K

Needle, yellow

$0.20 \times 0.05 \times 0.03$ mm

Data collection

Bruker SMART
diffractometer

φ and ω scans

Absorption correction: part of the refinement
model (ΔF)

(Walker & Stuart, 1983)

$T_{\min} = 0.298$, $T_{\max} = 0.456$

5556 measured reflections

5556 independent reflections

4453 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.097$

$\theta_{\max} = 28.9$ °, $\theta_{\min} = 1.6$ °

$h = -10 \rightarrow 12$

$k = -13 \rightarrow 8$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.077$

$S = 0.92$

5556 reflections

257 parameters

3 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$

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

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

$\Delta\rho_{\max} = 2.26$ e Å⁻³

$\Delta\rho_{\min} = -2.28$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.59034 (4)	0.85190 (3)	0.70913 (2)	0.01892 (7)
Au2	0.11598 (3)	0.01716 (3)	0.40500 (2)	0.02116 (8)
I1	0.85042 (7)	0.17524 (6)	0.33540 (4)	0.03085 (13)
I2	1.09742 (8)	0.86712 (6)	0.99527 (4)	0.03868 (15)
Fe1	0.58906 (12)	0.35008 (10)	0.69926 (7)	0.0154 (2)
O1	0.4739 (6)	0.3148 (6)	0.8300 (4)	0.0229 (11)
H1	0.379 (4)	0.310 (7)	0.825 (3)	0.034*
N4	0.8280 (7)	0.4651 (6)	0.8031 (4)	0.0197 (13)
N6	-0.1459 (9)	-0.2072 (8)	0.2275 (5)	0.0306 (16)
N2	0.3802 (7)	0.2347 (7)	0.5851 (4)	0.0206 (13)
N3	0.7137 (7)	0.3977 (6)	0.5585 (4)	0.0184 (12)
N7	0.8521 (8)	0.4547 (7)	0.3799 (5)	0.0252 (14)
C4	-0.0500 (9)	-0.1237 (9)	0.2898 (5)	0.0242 (16)
N8	1.1356 (8)	0.6149 (7)	0.9205 (5)	0.0270 (14)
N1	0.5698 (7)	0.5466 (6)	0.6996 (4)	0.0200 (12)
C3	0.2821 (9)	0.1544 (8)	0.5205 (5)	0.0186 (14)
N5	0.6142 (8)	1.1576 (7)	0.7088 (4)	0.0215 (13)
C6	0.8096 (9)	0.3307 (8)	0.4158 (5)	0.0196 (14)
C5	0.7384 (9)	0.2989 (8)	0.5038 (5)	0.0215 (15)
H5	0.707513	0.207434	0.525019	0.026*
C9	0.8752 (10)	0.5910 (8)	0.8594 (5)	0.0245 (16)
H9	0.802733	0.630763	0.860960	0.029*
C2	0.6042 (9)	1.0464 (8)	0.7107 (5)	0.0195 (14)
C8	0.7562 (9)	0.5225 (8)	0.5231 (5)	0.0223 (15)
H8	0.740253	0.594317	0.558402	0.027*
C1	0.5725 (9)	0.6564 (8)	0.7050 (5)	0.0211 (15)
C10	1.0299 (10)	0.6648 (8)	0.9160 (5)	0.0270 (18)
C7	0.8257 (10)	0.5510 (9)	0.4327 (6)	0.0289 (18)
H7	0.853931	0.641261	0.409642	0.035*
C12	0.9357 (9)	0.4135 (8)	0.8064 (5)	0.0227 (15)
H12	0.908739	0.325149	0.768484	0.027*
C11	1.0847 (10)	0.4878 (9)	0.8641 (6)	0.0271 (17)
H11	1.156693	0.447104	0.864451	0.033*
C13	0.4932 (10)	0.2326 (9)	0.9133 (5)	0.0290 (18)
H13A	0.603756	0.247389	0.930592	0.035*
H13B	0.428430	0.131598	0.889179	0.035*
C14	0.4467 (14)	0.2727 (13)	1.0106 (6)	0.055 (3)
H14A	0.340589	0.266687	0.992360	0.082*
H14B	0.519379	0.369119	1.039883	0.082*

H14C 0.449934 0.208333 1.062348 0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02856 (16)	0.01474 (13)	0.02017 (13)	0.01414 (12)	0.00870 (11)	0.00444 (10)
Au2	0.02192 (16)	0.02330 (14)	0.01917 (13)	0.00997 (12)	0.00570 (11)	0.00122 (11)
I1	0.0417 (3)	0.0313 (3)	0.0298 (2)	0.0205 (3)	0.0201 (2)	0.0053 (2)
I2	0.0482 (4)	0.0259 (3)	0.0367 (3)	0.0140 (3)	0.0020 (3)	-0.0082 (2)
Fe1	0.0220 (5)	0.0131 (4)	0.0152 (4)	0.0100 (4)	0.0070 (4)	0.0039 (4)
O1	0.026 (3)	0.032 (3)	0.018 (2)	0.018 (3)	0.008 (2)	0.007 (2)
N4	0.026 (3)	0.019 (3)	0.017 (3)	0.011 (3)	0.005 (2)	0.007 (2)
N6	0.033 (4)	0.044 (4)	0.025 (3)	0.024 (4)	0.010 (3)	0.003 (3)
N2	0.025 (4)	0.024 (3)	0.022 (3)	0.017 (3)	0.010 (3)	0.010 (3)
N3	0.021 (3)	0.022 (3)	0.017 (3)	0.012 (3)	0.010 (2)	0.008 (2)
N7	0.034 (4)	0.025 (3)	0.025 (3)	0.018 (3)	0.013 (3)	0.013 (3)
C4	0.027 (4)	0.036 (4)	0.023 (3)	0.025 (4)	0.010 (3)	0.001 (3)
N8	0.024 (4)	0.028 (3)	0.029 (3)	0.011 (3)	0.004 (3)	0.002 (3)
N1	0.023 (3)	0.017 (3)	0.022 (3)	0.010 (3)	0.004 (2)	0.004 (2)
C3	0.019 (4)	0.019 (3)	0.022 (3)	0.011 (3)	0.003 (3)	0.003 (3)
N5	0.025 (3)	0.020 (3)	0.023 (3)	0.011 (3)	0.011 (3)	0.004 (2)
C6	0.019 (4)	0.021 (3)	0.019 (3)	0.007 (3)	0.009 (3)	0.006 (3)
C5	0.025 (4)	0.022 (4)	0.018 (3)	0.009 (3)	0.008 (3)	0.004 (3)
C9	0.031 (4)	0.027 (4)	0.022 (3)	0.017 (4)	0.007 (3)	0.003 (3)
C2	0.023 (4)	0.020 (3)	0.023 (3)	0.014 (3)	0.010 (3)	0.002 (3)
C8	0.029 (4)	0.022 (4)	0.024 (3)	0.016 (3)	0.012 (3)	0.009 (3)
C1	0.024 (4)	0.021 (4)	0.023 (3)	0.013 (3)	0.008 (3)	0.002 (3)
C10	0.041 (5)	0.024 (4)	0.014 (3)	0.010 (4)	0.011 (3)	0.002 (3)
C7	0.040 (5)	0.026 (4)	0.032 (4)	0.018 (4)	0.024 (4)	0.019 (3)
C12	0.026 (4)	0.018 (3)	0.024 (3)	0.009 (3)	0.005 (3)	0.001 (3)
C11	0.030 (4)	0.033 (4)	0.026 (4)	0.021 (4)	0.005 (3)	0.004 (3)
C13	0.030 (5)	0.035 (4)	0.025 (4)	0.015 (4)	0.009 (3)	0.010 (3)
C14	0.060 (7)	0.086 (8)	0.024 (4)	0.032 (7)	0.017 (4)	0.011 (5)

Geometric parameters (Å, °)

Au1—Au2 ⁱ	3.163 (5)	N7—C7	1.309 (10)
Au1—C1	1.948 (9)	N8—C10	1.287 (11)
Au1—C2	1.952 (8)	N8—C11	1.329 (10)
Au2—C3	1.970 (8)	N1—C1	1.119 (10)
Au2—C4	1.981 (9)	N5—C2	1.111 (10)
I1—C6	2.071 (8)	C6—C5	1.387 (9)
I2—C10	2.078 (9)	C5—H5	0.9300
Fe1—O1	2.106 (6)	C9—H9	0.9300
Fe1—N1	2.105 (8)	C9—C10	1.384 (11)
Fe1—N2	2.096 (7)	C8—H8	0.9300
Fe1—N3	2.272 (7)	C8—C7	1.404 (10)
Fe1—N4	2.216 (7)	C7—H7	0.9300

Fe1—N5 ⁱⁱ	2.096 (8)	C12—H12	0.9300
O1—H1	0.859 (10)	C12—C11	1.350 (11)
O1—C13	1.419 (9)	C11—H11	0.9300
N4—C9	1.323 (10)	C13—H13A	0.9700
N4—C12	1.318 (10)	C13—H13B	0.9700
N6—C4	1.122 (10)	C13—C14	1.486 (11)
N2—C3	1.134 (9)	C14—H14A	0.9600
N3—C5	1.333 (9)	C14—H14B	0.9600
N3—C8	1.302 (9)	C14—H14C	0.9600
N7—C6	1.298 (9)		
C2—Au1—Au2 ⁱ	82.5 (2)	N7—C6—C5	123.1 (7)
C1—Au1—Au2 ⁱ	97.8 (2)	C5—C6—H1	119.6 (5)
C1—Au1—C2	178.8 (3)	N3—C5—C6	120.9 (7)
C4—Au2—Au1 ⁱ	101.9 (3)	N3—C5—H5	119.5
C3—Au2—Au1 ⁱ	78.1 (3)	C6—C5—H5	119.5
C3—Au2—C4	178.9 (3)	N4—C9—H9	119.3
O1—Fe1—N4	92.6 (3)	N4—C9—C10	121.4 (8)
O1—Fe1—N3	177.6 (2)	C10—C9—H9	119.3
N4—Fe1—N3	87.1 (3)	N5—C2—Au1	177.8 (7)
N2—Fe1—O1	94.9 (3)	N3—C8—H8	119.3
N2—Fe1—N4	171.7 (2)	N3—C8—C7	121.5 (7)
N2—Fe1—N3	85.6 (3)	C7—C8—H8	119.3
N2—Fe1—N1	95.8 (3)	N1—C1—Au1	175.8 (7)
N1—Fe1—O1	86.5 (2)	N8—C10—H2	118.1 (6)
N1—Fe1—N4	88.1 (3)	N8—C10—C9	123.0 (7)
N1—Fe1—N3	91.1 (2)	C9—C10—H2	118.9 (6)
N5 ⁱⁱ —Fe1—O1	91.3 (2)	N7—C7—C8	122.2 (7)
N5 ⁱⁱ —Fe1—N4	89.4 (3)	N7—C7—H7	118.9
N5 ⁱⁱ —Fe1—N2	87.0 (3)	C8—C7—H7	118.9
N5 ⁱⁱ —Fe1—N3	91.1 (2)	N4—C12—H12	119.7
N5 ⁱⁱ —Fe1—N1	176.6 (2)	N4—C12—C11	120.6 (7)
Fe1—O1—H1	122.0 (18)	C11—C12—H12	119.7
C13—O1—Fe1	126.0 (5)	N8—C11—C12	124.5 (8)
C13—O1—H1	105.7 (18)	N8—C11—H11	117.8
C9—N4—Fe1	123.4 (5)	C12—C11—H11	117.8
C12—N4—Fe1	120.4 (5)	O1—C13—H13A	109.3
C12—N4—C9	116.1 (7)	O1—C13—H13B	109.3
C3—N2—Fe1	165.9 (6)	O1—C13—C14	111.7 (8)
C5—N3—Fe1	122.6 (5)	H13A—C13—H13B	107.9
C8—N3—Fe1	120.9 (5)	C14—C13—H13A	109.3
C8—N3—C5	116.4 (6)	C14—C13—H13B	109.3
C6—N7—C7	116.0 (6)	C13—C14—H14A	109.5
N6—C4—Au2	177.2 (7)	C13—C14—H14B	109.5
C10—N8—C11	114.3 (7)	C13—C14—H14C	109.5
C1—N1—Fe1	174.0 (6)	H14A—C14—H14B	109.5
N2—C3—Au2	178.2 (6)	H14A—C14—H14C	109.5
C2—N5—Fe1 ⁱⁱⁱ	169.9 (7)	H14B—C14—H14C	109.5

N7—C6—I1	117.3 (5)		
I1—C6—C5—N3	178.6 (5)	C6—N7—C7—C8	0.3 (12)
Fe1—O1—C13—C14	158.4 (6)	C5—N3—C8—C7	-0.6 (11)
Fe1—N4—C9—C10	-174.4 (5)	C9—N4—C12—C11	-0.3 (10)
Fe1—N4—C12—C11	175.7 (5)	C8—N3—C5—C6	1.6 (10)
Fe1—N3—C5—C6	177.5 (5)	C10—N8—C11—C12	-0.3 (11)
Fe1—N3—C8—C7	-176.6 (6)	C7—N7—C6—I1	-179.6 (6)
N4—C9—C10—I2	176.5 (5)	C7—N7—C6—C5	0.8 (11)
N4—C9—C10—N8	-2.2 (11)	C12—N4—C9—C10	1.5 (10)
N4—C12—C11—N8	-0.3 (12)	C11—N8—C10—I2	-177.3 (5)
N3—C8—C7—N7	-0.4 (13)	C11—N8—C10—C9	1.5 (10)
N7—C6—C5—N3	-1.8 (11)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N6 ^{iv}	0.86 (5)	1.98 (5)	2.765 (13)	151 (6)

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