



Crystal structure of *catena*-poly[[[diaqua[1,2-bis(pyridin-4-yl)ethene]{4-[2-(pyridin-4-yl)ethenyl]-pyridinium}gold(I)iron(II)]-di- μ -cyanido] bis[dicyanidogold(I)] 1,2-bis(pyridin-4-yl)ethene dihydrate]

Sofiia V. Partsevskaya,^{a*} Dina D. Naumova,^a Igor P. Matushko,^a Sergiu Shova^b and Il'ya A. Gural'skiy^{a,c}

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^aDepartment of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska St. 64, Kyiv 01601, Ukraine,

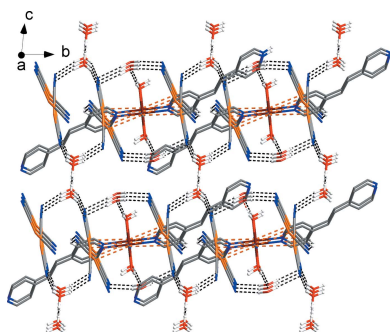
^bDepartment of Inorganic Polymers, "Petru Poni" Institute of Macromolecular Chemistry, Romanian Academy of Science, Aleea Grigore Ghica Voda 41-A, Iasi 700487, Romania, and ^cUkrOrgSyntez Ltd, Chervonotkatska St., 67, Kyiv 02094, Ukraine. *Correspondence e-mail: sofiia.partsevskaya@univ.kiev.ua

In the title compound $[\text{Fe}(\text{bpe})(\text{Hbpe})\text{Au}(\text{CN})_2][\text{Au}(\text{CN})_2]_2 \cdot \text{bpe} \cdot 2\text{H}_2\text{O}]_n$ [where $\text{bpe} = 1,2\text{-bis}(\text{pyridin-4-yl})\text{ethene}$, $\text{C}_{12}\text{H}_{10}\text{N}_2$], the Fe^{II} ion is coordinated in a distorted octahedral $[\text{FeN}_4\text{O}_2]$ environment by two dicyanoaurate anions, two water molecules and two partially protonated 1,2-di(4-pyridyl)ethylene molecules. Dicyanoaurate anions bridge the Fe^{II} cations, forming infinite chains, which propagate along the *a*-axis direction. The chains are connected *via* aurophilic interactions with two non-coordinated dicyanoaurate anions for each Fe^{II} ion. The polymeric chains interact with each other *via* π - π stacking between the guest *bpe* molecules and multiple hydrogen bonds.

1. Chemical context

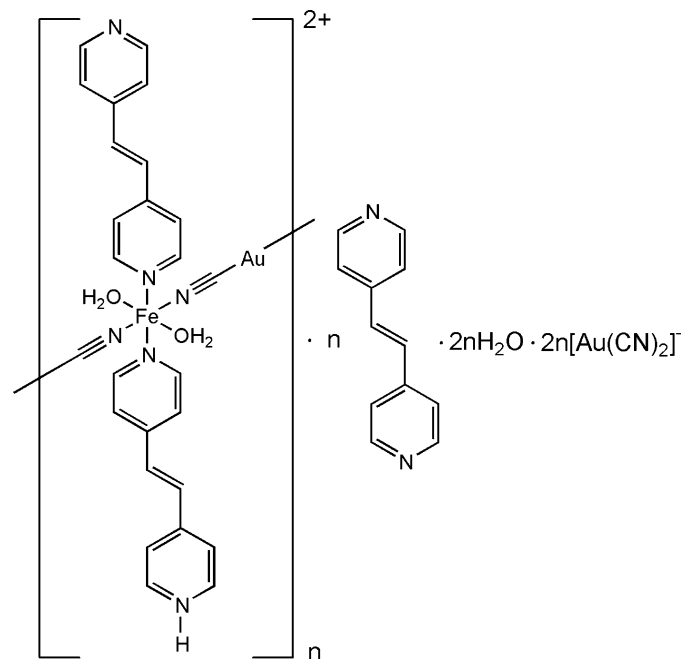
Iron(II) complexes exhibiting spin-crossover (SCO) properties attract considerable attention because of their fascinating ability to change multiple physical properties (magnetic, optical, mechanical, *etc.*) under the influence of external stimuli (Gütlich & Goodwin, 2004). These materials can be integrated into various devices as switches, triggers, chemical sensors, *etc.* (Suleimanov *et al.*, 2015). For these reasons, new SCO materials, which undergo transition with defined temperature, hysteresis and abruptness are strongly desired. There are several classical approaches as how to modulate the SCO characteristics of complexes, among them the introduction of slightly modified ligands and co-ligands to obtain new SCO compounds and inclusion of some guest molecules to already existing complexes (Ni *et al.*, 2017).

Fe^{II} Hofmann clathrate (Hofmann & Höchtlen, 1903) analogues represent one of the biggest classes of SCO coordination compounds. They are cyanobimetallic complexes of general formula $[\text{Fe}(L)_n\{M(\text{CN})_x\}_y]$ in which the Fe^{II} ions are connected by bridging cyanometallic anions into infinite layers ($n = 2$ for monodentate ligands and $n = 1$ for bis-monodentate ligands). These layers are supported by N-donor aromatic ligands ($L = \text{pyridine}$, diazines and their substituted analogues). Di-, tetra- and octacyanometallic ($x = 2, y = 2$: $M = \text{Cu}, \text{Ag}, \text{Au}$; $x = 4, y = 1$: $M = \text{Ni}, \text{Pd}, \text{Pt}$) anions have been introduced to develop coordination compounds of this kind. It has been shown that the inclusion of guest molecules can



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significantly influence the temperature, completeness and step character of spin transition in complexes belonging to this class (Ohtani & Hayami, 2017). In order to develop new SCO Hofmann clathrate analogues with voids big enough to incorporate bulky guest molecules, some bis-monodentate pyridine-based ligands have been introduced, such as 4,4'-bipyridine (Yoshida *et al.*, 2013), bis(4-pyridyl)acetylene (Bartual-Murgui *et al.*, 2011), bis(4-pyridyl)ethylene (Muñoz-Lara *et al.*, 2012), *etc.*



Here we describe the crystal structure of a new cyanometallic Fe^{II} complex with bpe of general formula [Fe(bpe)(Hbpe)Au(CN)₂](Au(CN)₂)₂·bpe·2H₂O in which the Fe^{II} ions are stabilized in the high-spin (HS) state.

2. Structural commentary

The title compound crystallizes in the triclinic $P\bar{1}$ space group. The iron(II) ion has a distorted [FeN₄O₂] octahedral environment (Fig. 1) formed by two molecules of 1,2-bis(4-pyridyl)ethylene (bpe) [Fe1–N4 = 2.223 (6) Å], two molecules of water [Fe1–O1 = 2.081 (5) Å] and two cyano bridges [Fe1–N1 = 2.180 (6) Å]. Notably, the N5 atoms of the coordinated bpe molecules are protonated (with 0.5 occupancy of each H atom). These N5 atoms create hydrogen bonds with symmetry-generated N5 atoms of bpe molecules from the neighbouring chain [N5···N5ⁱ = 2.677 (14) Å, N5–H5A···N5ⁱ = 176°; Table 1].

The deviation from the ideal octahedral geometry of the Fe^{II} coordination environment is $\Sigma|90 - \theta| = 6.8^\circ$, where θ are *cis*-N–Fe–N or *cis*-N–Fe–O angles. Two CN[−] anions bridge the Fe²⁺ and Au⁺ cations [Fe1···Au1 = 5.280 (3) Å], creating a one-dimensional polymer, Fe1–N1–C1 = 172.8 (7)°, N1–C1–Au1 = 179.1 (8)° and C1–Au1–C1 = 180.0°, leading to a very slight deviation from linearity of the

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

D–H···A	D–H	H···A	D···A	D–H···A
O1–H1A···O2	0.93	1.86	2.744 (13)	156
O1–H1B···N6	0.93	1.85	2.736 (9)	158
C7–H7···N2B	0.93	2.08	2.78 (3)	132
N5–H5A···N5 ⁱ	0.86	1.82	2.677 (14)	176
O2–H2A···N2A ⁱⁱ	0.96	2.49	3.45 (7)	179
O2–H2B···N3B ⁱⁱⁱ	0.94	2.43	3.37 (3)	172
O3–H3B···N3A	0.92	2.08	2.99 (3)	167
O3–H3A···N2A ^{iv}	0.92	2.11	2.98 (4)	159
O3–H3C···O3 ^v	0.94	1.75	2.69 (4)	179

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

chains. This chain binds one guest bpe and two guest water molecules per Fe^{II} centre.

3. Supramolecular features

The structure is characterized by the presence of several different kinds of weak interactions that create a three-dimensional supramolecular framework. Two free [Au(CN)₂][−] counter-ions are connected with the polymeric chains by aurophilic interactions and C7···N2B hydrogen bonds [C7···N2B = 2.78 (3) Å, C7–H7···N2B = 132°]. These free counter-ions are disordered over two positions with Au1–Au2A = 3.324 (1) Å and Au1–Au2B = 3.101 (5) Å. The polymeric chains are connected to each other *via* π – π interactions (Fig. 2) between the coordinated and guest molecules of bpe (Cg1···Cg2 = 3.650 (5) Å, $\alpha = 10.3^\circ$, offset = 1.043 Å, where Cg1 and Cg2 are the centroids of the N4/C4–C8 and N6/C16–C20 rings, respectively, and Cg3···Cg4 = 3.794 (6) Å, $\alpha = 6.8^\circ$, offset = 1.835 Å, where Cg3 and Cg4 are the centroids of N5/C11–C15 and N6ⁱⁱ/Cⁱⁱⁱ16–C20 rings, respectively). Guest bpe molecules are additionally linked to the polymeric chains by hydrogen bonds with coordinated water molecules [O1···N6 = 2.736 (9) Å, O1–H1B···N6 = 158°]. One of the guest water molecules forms hydrogen bonds with the coordinated water [Fig. 3; O2···O1 = 2.744 (13) Å, O1–

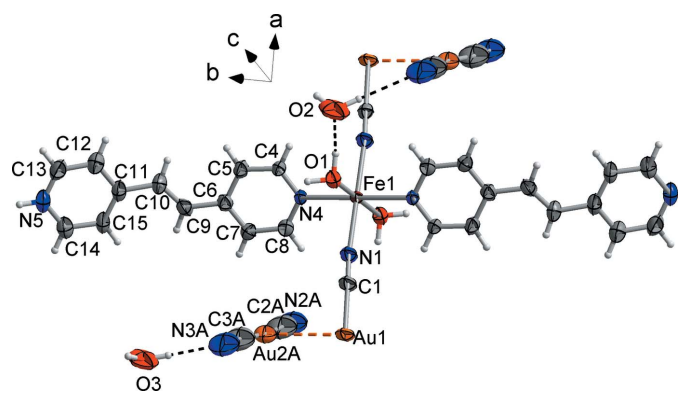
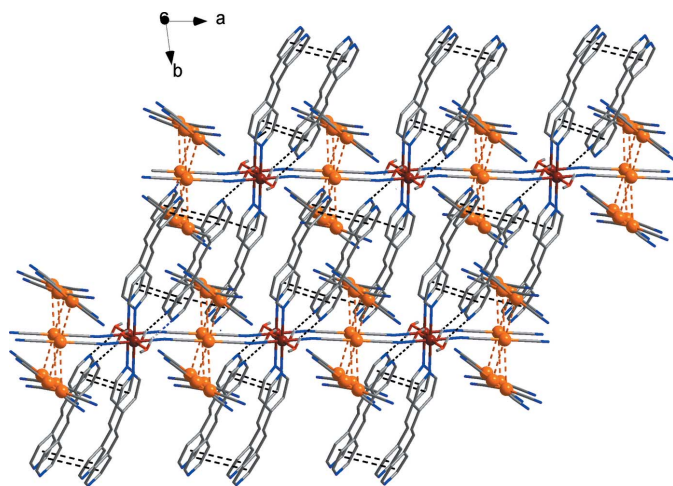


Figure 1
A fragment of the crystal structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The guest bpe molecule and disorder of the [Au(CN)₂][−] counter-ions are not shown for clarity. Symmetry-generated atoms are not labelled.


Figure 2

A view along the c axis of the crystal packing of the title compound. π - π contacts and hydrogen bonds are shown as black dashed lines. Aurophilic interactions are shown as orange dashed lines. Guest water molecules are omitted for clarity.

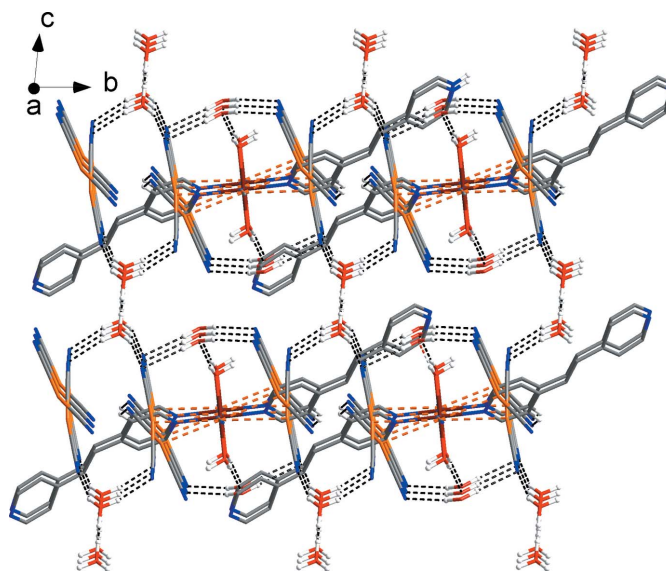
$H1A \cdots O2 = 156^\circ$] and weak hydrogen bonds with free dicyanoaurate counter-ions [$O2 \cdots N2A^{ii} = 3.45(7) \text{ \AA}$, $O2-H2A \cdots N2A^{ii} = 179^\circ$; $O2 \cdots N3B^{iii} = 3.37(3) \text{ \AA}$, $O2-H2B \cdots N3B^{iii} = 172^\circ$. The $O3$ guest water atom is bound to another symmetry-generated counterpart [$O3 \cdots O3^v = 2.69(4) \text{ \AA}$, $O3-H3C \cdots O3^v = 179^\circ$] and free dicyanoaurate counter-ions [$O3 \cdots N3A = 2.99(3) \text{ \AA}$, $O3-H3B \cdots N3A = 167^\circ$; $O3 \cdots N2A^{iv} = 2.98(4) \text{ \AA}$, $O3-H3A \cdots N2A^{iv} = 159^\circ$]. Hydrogen-bonding parameters are summarized in Table 1.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.40, last update February 2019; Groom *et al.*, 2016) revealed that the current structure has never been published before. 101 cyanometallic structures containing $Fe-N \equiv C-Au$ fragments were found. These hits include multiple temperature-dependant measurements, which were conducted to study the spin-crossover characteristics of Fe^{II} complexes. For example, these hits include a three-dimensional framework *catena*-[tetra(μ -cyano)(μ -pyrazine)iron(II)gold(I)] (IRIKUR01-IRIKUR09; Gural'skiy *et al.*, 2016). One particular compound resembles the title MOF: *catena*-[bis(μ -cyano)bis(2-phenylpyrazine)bis(aqua)iron(II)gold(I) bis(cyano)gold(I)] (MOJ-FEZ; Kucheriv *et al.*, 2019).

5. Synthesis and crystallization

Crystals of the title compound were prepared by the slow diffusion method between three layers in a 3 ml tube. The first layer was a solution of $K[Au(CN)_2]$ (0.03 mmol) in water (0.5 ml), the second was a mixture of water/ethanol (1:2, 1.5 ml) and the third layer was a solution of 1,2-di(4-pyridyl)ethylene (0.05 mmol) and $[Fe(OTs)_2] \cdot 6H_2O$ (0.01 mmol; OTs = *p*-toluenesulfonate) in ethanol (0.5 ml) with 0.2 ml of water. After two weeks, red crystals grew in the second layer;


Figure 3

A view along the a axis of the crystal packing showing the network of hydrogen bonds as black dashed lines. H atoms not involved in hydrogen bonding and guest bpe molecules are omitted for clarity.

the crystals were collected and kept in the mother solution prior to measurement.

Table 2

Experimental details.

Crystal data	
Chemical formula	$[AuFe(C_{12}H_{11}N_2)(CN)_2-(C_{12}H_{10}N_2)][Au(CN)_2]_2 \cdot C_{12}H_{10}N_2 \cdot 2H_2O$
M_r	1422.60
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	10.5601 (7), 11.0044 (12), 11.8145 (10)
α, β, γ ($^\circ$)	80.212 (8), 69.124 (7), 78.565 (7)
V (Å ³)	1249.9 (2)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	9.11
Crystal size (mm)	0.4 × 0.3 × 0.2
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, Eos
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)
T_{min}, T_{max}	0.350, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9662, 4402, 3540
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.156, 1.04
No. of reflections	4402
No. of parameters	272
No. of restraints	9
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	2.27, -1.04

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were placed at their expected calculated positions ($C-H = 0.93$, $N-H = 0.86$, $O-H = 0.92-0.96$ Å) and refined as riding for the guest water molecules (O2, O3) and aromatic rings, and as rotating for the coordinated water molecule (O1) with $U_{iso}(H) = 1.2U_{iso}(C)$, $U_{iso}(H) = 1.2U_{iso}(N)$, $U_{iso}(H) = 1.5U_{iso}(O)$. U_{aniso} values for all C and N atoms in the guest dicyanoaurate anions and the O2 and O3 water molecules were constrained to be equal using the EADP command. Distances $N3A-C3A$ and $N2A-C2A$ were restrained to a target of 1.15 Å and distances $Au2A-C3A$ and $Au2A-C2A$ were restrained to a target of 1.99 Å using the DFIX command. The following distances were restrained to be equal using the SADI command: $C2A-N2A$ and $C2B-N2B$; $Au1-C2A$ and $Au1-C2B$; $C3A-N3A$ and $C3B-N3B$; $Au1-C3A$ and $Au1-C3B$; $C2A-C3A$ and $C2B-C3B$.

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References

- Bartual-Murgui, C., Ortega-Villar, N. A., Shepherd, H. J., Muñoz, M. C. C., Salmon, L., Molnár, G., Bousseksou, A. & Real, J. A. (2011). *J. Mater. Chem.* **21**, 7217–7222.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Gural'skiy, I. A., Golub, B. O., Shylin, S. I., Ksenofontov, V., Shepherd, H. J., Raithby, P. R., Tremel, W. & Fritsky, I. O. (2016). *Eur. J. Inorg. Chem.* pp. 3191–3195.
- Gütlich, P. & Goodwin, H. A. (2004). *Spin Crossover in Transition Metal Compounds I*, pp. 1–47. Berlin, Heidelberg: Springer-Verlag.
- Hofmann, K. A. & Höchtlen, F. (1903). *Ber. Dtsch. Chem. Ges.* **36**, 1149–1151.
- Kucheriv, O. I., Barakhtii, D. D., Malinkin, S. O., Shova, S. & Gural'skiy, I. A. (2019). *Acta Cryst.* **E75**, 1149–1152.
- Muñoz-Lara, F. J., Gaspar, A. B., Muñoz, M. C., Arai, M., Kitagawa, S., Ohba, M. & Real, J. A. (2012). *Chem. Eur. J.* **18**, 8013–8018.
- Ni, Z.-P., Liu, J.-L., Hoque, M. N., Liu, W., Li, J.-Y., Chen, Y.-C. & Tong, M.-L. (2017). *Coord. Chem. Rev.* **335**, 28–43.
- Ohtani, R. & Hayami, S. (2017). *Chem. Eur. J.* **23**, 2236–2248.
- Rigaku OD (2016). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Suleimanov, I., Kraieva, O., Sánchez Costa, J., Fritsky, I. O., Molnár, G., Salmon, L. & Bousseksou, A. (2015). *J. Mater. Chem. C* **3**, 5026–5032.
- Yoshida, K., Akahoshi, D., Kawasaki, T., Saito, T. & Kitazawa, T. (2013). *Polyhedron*, **66**, 252–256.

supporting information

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Crystal structure of *catena*-poly[[[diaqua[1,2-bis(pyridin-4-yl)ethene]{4-[2-(pyridin-4-yl)ethenyl]pyridinium}gold(I)iron(II)]-di- μ -cyanido] bis[dicyanidogold(I)] 1,2-bis(pyridin-4-yl)ethene dihydrate]

Sofia V. Partsevskaya, Dina D. Naumova, Igor P. Matushko, Sergiu Shova and Il'ya A. Gural'skiy

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

catena-Poly[[[diaqua[1,2-bis(pyridin-4-yl)ethene]{4-[2-(pyridin-4-yl)ethenyl]pyridinium}gold(I)iron(II)]-di- μ -cyanido] bis[dicyanidogold(I)] 1,2-bis(pyridin-4-yl)ethene dihydrate]

Crystal data

[AuFe(C₁₂H₁₁N₂)(CN)₂(C₁₂H₁₀N₂)]
 [Au(CN)₂]₂·C₁₂H₁₀N₂·2H₂O
M_r = 1422.60
 Triclinic, *P* $\bar{1}$
a = 10.5601 (7) Å
b = 11.0044 (12) Å
c = 11.8145 (10) Å
 α = 80.212 (8)°
 β = 69.124 (7)°
 γ = 78.565 (7)°
V = 1249.9 (2) Å³

Z = 1
F(000) = 670
D_x = 1.890 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 3572 reflections
 θ = 1.9–27.9°
 μ = 9.11 mm⁻¹
T = 293 K
 Block, red
 0.4 × 0.3 × 0.2 mm

Data collection

Rigaku Oxford Diffraction Xcalibur, Eos diffractometer
 Detector resolution: 8.0797 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.350, *T_{max}* = 1.000
 9662 measured reflections

4402 independent reflections
 3540 reflections with *I* > 2 σ (*I*)
R_{int} = 0.042
 θ_{\max} = 25.0°, θ_{\min} = 1.9°
h = -11→12
k = -13→12
l = -11→14

Refinement

Refinement on *F*²
 Least-squares matrix: full
R [*F*² > 2 σ (*F*²)] = 0.050
wR(*F*²) = 0.156

S = 1.03
 4402 reflections
 272 parameters
 9 restraints

Hydrogen site location: mixed
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0855P)^2 + 0.8591P]$
 where $P = (F_o^2 + 2F_c^2)/3$

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

$$\Delta\rho_{\max} = 2.27 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.04 \text{ e } \text{\AA}^{-3}$$

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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Au1	1.000000	0.000000	-0.500000	0.0441 (2)	
Fe1	1.500000	0.000000	-0.500000	0.0292 (4)	
N6	1.2335 (8)	0.1426 (7)	-0.1913 (6)	0.0501 (18)	
O1	1.4274 (5)	-0.0394 (6)	-0.3113 (5)	0.0438 (14)	
H1A	1.496163	-0.065149	-0.276444	0.066*	
H1B	1.381652	0.030289	-0.270914	0.066*	
C8	1.3795 (8)	0.2828 (8)	-0.5220 (7)	0.0423 (19)	
H8	1.353283	0.259226	-0.581414	0.051*	
C5	1.4616 (8)	0.3566 (8)	-0.3576 (8)	0.043 (2)	
H5	1.495858	0.380110	-0.303466	0.052*	
C4	1.5067 (7)	0.2397 (8)	-0.3988 (7)	0.0395 (19)	
H4	1.570087	0.185167	-0.369306	0.047*	
C18	1.0834 (8)	0.3621 (9)	-0.0954 (8)	0.048 (2)	
N4	1.4646 (6)	0.2017 (6)	-0.4772 (5)	0.0317 (14)	
C21	0.9996 (10)	0.4782 (10)	-0.0484 (8)	0.055 (2)	
H21	0.942320	0.523726	-0.089865	0.066*	
C9	1.2973 (8)	0.5573 (8)	-0.3485 (8)	0.044 (2)	
H9	1.240584	0.609573	-0.386971	0.053*	
C17	1.1829 (10)	0.2903 (10)	-0.0506 (8)	0.059 (3)	
H17	1.201690	0.315099	0.012449	0.071*	
N1	1.2923 (6)	0.0142 (7)	-0.5030 (6)	0.0433 (17)	
C19	1.0669 (9)	0.3182 (10)	-0.1910 (8)	0.052 (2)	
H19	1.003778	0.363330	-0.226531	0.063*	
C20	1.1418 (9)	0.2094 (9)	-0.2342 (9)	0.055 (2)	
H20	1.126215	0.181889	-0.297643	0.065*	
C6	1.3638 (8)	0.4388 (8)	-0.3989 (7)	0.0412 (19)	
C11	1.2282 (9)	0.7084 (8)	-0.1962 (8)	0.048 (2)	
C7	1.3274 (8)	0.4002 (8)	-0.4855 (7)	0.0415 (19)	
H7	1.267286	0.453324	-0.519895	0.050*	
C15	1.1322 (10)	0.7868 (9)	-0.2320 (9)	0.057 (3)	
H15	1.116876	0.775000	-0.301887	0.069*	
C10	1.3093 (9)	0.5968 (8)	-0.2560 (8)	0.047 (2)	
H10	1.375191	0.550547	-0.224182	0.057*	
N5	1.0744 (8)	0.9079 (7)	-0.0674 (7)	0.0513 (19)	
H5A	1.025191	0.968647	-0.026905	0.062*	0.5

C1	1.1866 (8)	0.0083 (8)	-0.5027 (7)	0.0413 (19)	
C13	1.1698 (10)	0.8351 (10)	-0.0344 (9)	0.061 (3)	
H13	1.185868	0.851036	0.033766	0.073*	
C12	1.2496 (10)	0.7344 (9)	-0.0949 (9)	0.057 (2)	
H12	1.317168	0.684662	-0.067302	0.069*	
C16	1.2541 (9)	0.1809 (10)	-0.1014 (9)	0.058 (3)	
H16	1.319389	0.132921	-0.069841	0.070*	
C14	1.0551 (11)	0.8852 (10)	-0.1667 (9)	0.064 (3)	
H14	0.987822	0.937040	-0.193066	0.077*	
N3A	0.7442 (6)	0.2821 (9)	-0.2440 (3)	0.140 (5)	0.8
C3A	0.8293 (4)	0.2875 (6)	-0.3312 (2)	0.140 (5)	0.8
Au2A	0.96785 (10)	0.30552 (9)	-0.49275 (9)	0.1010 (3)	0.8
C2A	1.1004 (4)	0.3499 (6)	-0.6389 (3)	0.140 (5)	0.8
N2A	1.1797 (6)	0.3786 (9)	-0.7294 (4)	0.140 (5)	0.8
N3B	0.703 (3)	0.119 (3)	-0.1529 (17)	0.140 (5)	0.2
C3B	0.7686 (18)	0.1679 (19)	-0.2399 (12)	0.140 (5)	0.2
Au2B	0.8855 (5)	0.2557 (4)	-0.3973 (6)	0.151 (2)	0.2
C2B	1.010 (2)	0.3636 (18)	-0.4940 (14)	0.140 (5)	0.2
N2B	1.095 (3)	0.424 (3)	-0.552 (2)	0.140 (5)	0.2
O2	1.5706 (15)	-0.1345 (17)	-0.1543 (12)	0.109 (5)	0.6
H2A	1.640962	-0.201711	-0.187906	0.164*	0.6
H2B	1.609492	-0.067311	-0.147186	0.164*	0.6
O3	0.574 (2)	0.503 (3)	-0.1194 (19)	0.109 (5)	0.4
H3B	0.617417	0.427938	-0.148163	0.164*	0.2
H3A	0.637317	0.556568	-0.154373	0.164*	0.4
H3C	0.522617	0.501478	-0.035993	0.164*	0.2

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0232 (2)	0.0500 (3)	0.0655 (4)	-0.00604 (19)	-0.0212 (2)	-0.0086 (2)
Fe1	0.0194 (7)	0.0277 (9)	0.0434 (8)	-0.0019 (6)	-0.0110 (6)	-0.0127 (6)
N6	0.056 (4)	0.038 (5)	0.048 (4)	-0.004 (4)	-0.005 (4)	-0.012 (3)
O1	0.041 (3)	0.045 (4)	0.044 (3)	0.005 (3)	-0.013 (3)	-0.014 (3)
C8	0.041 (4)	0.041 (5)	0.047 (5)	-0.003 (4)	-0.014 (4)	-0.015 (4)
C5	0.042 (4)	0.036 (5)	0.054 (5)	-0.009 (4)	-0.013 (4)	-0.017 (4)
C4	0.034 (4)	0.035 (5)	0.055 (5)	0.000 (3)	-0.019 (4)	-0.020 (4)
C18	0.037 (4)	0.045 (6)	0.051 (5)	-0.013 (4)	0.003 (4)	-0.011 (4)
N4	0.029 (3)	0.024 (4)	0.044 (4)	0.000 (3)	-0.014 (3)	-0.011 (3)
C21	0.052 (5)	0.048 (6)	0.065 (6)	-0.003 (4)	-0.014 (5)	-0.024 (5)
C9	0.035 (4)	0.031 (5)	0.065 (6)	0.000 (3)	-0.016 (4)	-0.008 (4)
C17	0.064 (6)	0.072 (8)	0.046 (5)	-0.012 (5)	-0.016 (5)	-0.021 (5)
N1	0.030 (3)	0.037 (4)	0.066 (5)	-0.004 (3)	-0.018 (3)	-0.011 (3)
C19	0.052 (5)	0.059 (7)	0.042 (5)	-0.006 (5)	-0.011 (4)	-0.009 (4)
C20	0.054 (5)	0.051 (6)	0.057 (6)	-0.010 (5)	-0.010 (5)	-0.019 (5)
C6	0.031 (4)	0.041 (5)	0.050 (5)	-0.004 (3)	-0.008 (3)	-0.014 (4)
C11	0.048 (5)	0.037 (5)	0.055 (5)	-0.009 (4)	-0.006 (4)	-0.019 (4)
C7	0.042 (4)	0.036 (5)	0.051 (5)	-0.005 (4)	-0.021 (4)	-0.008 (4)

C15	0.071 (6)	0.041 (6)	0.065 (6)	0.009 (5)	-0.027 (5)	-0.029 (5)
C10	0.056 (5)	0.034 (5)	0.055 (5)	-0.003 (4)	-0.018 (4)	-0.016 (4)
N5	0.056 (5)	0.039 (5)	0.053 (4)	-0.004 (4)	-0.006 (4)	-0.020 (4)
C1	0.026 (4)	0.043 (5)	0.054 (5)	-0.005 (3)	-0.012 (4)	-0.008 (4)
C13	0.058 (6)	0.064 (7)	0.066 (6)	-0.014 (5)	-0.016 (5)	-0.031 (5)
C12	0.064 (6)	0.047 (6)	0.065 (6)	-0.004 (5)	-0.022 (5)	-0.021 (5)
C16	0.047 (5)	0.057 (7)	0.062 (6)	0.008 (5)	-0.014 (5)	-0.014 (5)
C14	0.075 (7)	0.046 (7)	0.076 (7)	0.010 (5)	-0.033 (6)	-0.024 (5)
N3A	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
C3A	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
Au2A	0.1098 (6)	0.0872 (7)	0.1463 (8)	0.0284 (5)	-0.0985 (6)	-0.0475 (5)
C2A	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
N2A	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
N3B	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
C3B	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
Au2B	0.174 (4)	0.092 (3)	0.276 (6)	0.037 (3)	-0.186 (5)	-0.081 (4)
C2B	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
N2B	0.181 (11)	0.132 (9)	0.155 (11)	0.018 (9)	-0.130 (10)	-0.026 (9)
O2	0.101 (10)	0.146 (14)	0.087 (8)	0.033 (9)	-0.066 (7)	-0.010 (8)
O3	0.101 (10)	0.146 (14)	0.087 (8)	0.033 (9)	-0.066 (7)	-0.010 (8)

Geometric parameters (Å, °)

Au1—C1 ⁱ	1.979 (7)	N1—C1	1.130 (10)
Au1—C1	1.979 (7)	C19—H19	0.9300
Au1—Au2A	3.3243	C19—C20	1.366 (13)
Au1—Au2A ⁱ	3.3243	C20—H20	0.9300
Au1—Au2B	3.101 (4)	C6—C7	1.367 (11)
Au1—Au2B ⁱ	3.101 (4)	C11—C15	1.336 (13)
Fe1—O1 ⁱⁱ	2.081 (5)	C11—C10	1.479 (11)
Fe1—O1	2.081 (5)	C11—C12	1.379 (12)
Fe1—N4	2.223 (6)	C7—H7	0.9300
Fe1—N4 ⁱⁱ	2.223 (6)	C15—H15	0.9300
Fe1—N1 ⁱⁱ	2.180 (6)	C15—C14	1.385 (12)
Fe1—N1	2.181 (6)	C10—H10	0.9300
N6—C20	1.294 (12)	N5—H5A	0.8600
N6—C16	1.307 (12)	N5—C13	1.290 (12)
O1—H1A	0.9319	N5—C14	1.330 (12)
O1—H1B	0.9285	C13—H13	0.9300
C8—H8	0.9300	C13—C12	1.385 (13)
C8—N4	1.320 (10)	C12—H12	0.9300
C8—C7	1.377 (11)	C16—H16	0.9300
C5—H5	0.9300	C14—H14	0.9300
C5—C4	1.387 (11)	N3A—C3A	1.1014
C5—C6	1.401 (12)	C3A—Au2A	1.9543
C4—H4	0.9300	Au2A—C2A	1.8554
C4—N4	1.315 (9)	C2A—N2A	1.1381
C18—C21	1.472 (13)	N3B—C3B	1.1270

C18—C17	1.390 (13)	C3B—Au2B	2.0356
C18—C19	1.377 (12)	Au2B—C2B	1.8767
C21—C21 ⁱⁱⁱ	1.317 (17)	C2B—N2B	1.1712
C21—H21	0.9300	O2—H2A	0.9640
C9—H9	0.9300	O2—H2B	0.9427
C9—C6	1.466 (11)	O3—H3B	0.9225
C9—C10	1.298 (11)	O3—H3A	0.9170
C17—H17	0.9300	O3—H3C	0.9389
C17—C16	1.393 (13)		
C1 ⁱ —Au1—C1	180.0	C16—C17—H17	120.4
C1 ⁱ —Au1—Au2A	98.7 (3)	C1—N1—Fe1	172.8 (7)
C1—Au1—Au2A	81.3 (3)	C18—C19—H19	119.5
C1—Au1—Au2A ⁱ	98.7 (14)	C20—C19—C18	121.0 (9)
C1 ⁱ —Au1—Au2A ⁱ	81.3 (14)	C20—C19—H19	119.5
C1 ⁱ —Au1—Au2B	88.0 (3)	N6—C20—C19	123.2 (9)
C1—Au1—Au2B	92.0 (3)	N6—C20—H20	118.4
C1 ⁱ —Au1—Au2B ⁱ	92 (3)	C19—C20—H20	118.4
C1—Au1—Au2B ⁱ	88 (3)	C5—C6—C9	122.6 (7)
Au2A ⁱ —Au1—Au2A	180.0 (18)	C7—C6—C5	116.4 (8)
Au2B—Au1—Au2B ⁱ	180 (5)	C7—C6—C9	120.9 (8)
O1 ⁱⁱ —Fe1—O1	180.0	C15—C11—C10	124.7 (8)
O1 ⁱⁱ —Fe1—N4 ⁱⁱ	89.1 (2)	C15—C11—C12	116.4 (9)
O1—Fe1—N4	89.1 (2)	C12—C11—C10	118.9 (9)
O1 ⁱⁱ —Fe1—N4	90.9 (2)	C8—C7—H7	119.9
O1—Fe1—N4 ⁱⁱ	90.9 (2)	C6—C7—C8	120.1 (8)
O1—Fe1—N1 ⁱⁱ	90.4 (2)	C6—C7—H7	119.9
O1—Fe1—N1	89.6 (2)	C11—C15—H15	119.5
O1 ⁱⁱ —Fe1—N1 ⁱⁱ	89.6 (2)	C11—C15—C14	121.1 (9)
O1 ⁱⁱ —Fe1—N1	90.4 (2)	C14—C15—H15	119.5
N4—Fe1—N4 ⁱⁱ	180.0	C9—C10—C11	126.2 (9)
N1 ⁱⁱ —Fe1—N4	89.6 (2)	C9—C10—H10	116.9
N1 ⁱⁱ —Fe1—N4 ⁱⁱ	90.4 (2)	C11—C10—H10	116.9
N1—Fe1—N4 ⁱⁱ	89.6 (2)	C13—N5—H5A	121.4
N1—Fe1—N4	90.4 (2)	C13—N5—C14	117.3 (8)
N1 ⁱⁱ —Fe1—N1	180.0	C14—N5—H5A	121.4
C20—N6—C16	118.2 (8)	N1—C1—Au1	179.0 (8)
Fe1—O1—H1A	114.1	N5—C13—H13	118.2
Fe1—O1—H1B	113.4	N5—C13—C12	123.5 (9)
H1A—O1—H1B	100.1	C12—C13—H13	118.2
N4—C8—H8	118.2	C11—C12—C13	119.6 (9)
N4—C8—C7	123.6 (7)	C11—C12—H12	120.2
C7—C8—H8	118.2	C13—C12—H12	120.2
C4—C5—H5	120.5	N6—C16—C17	123.0 (9)
C4—C5—C6	119.0 (7)	N6—C16—H16	118.5
C6—C5—H5	120.5	C17—C16—H16	118.5
C5—C4—H4	118.2	C15—C14—H14	119.0
N4—C4—C5	123.5 (8)	N5—C14—C15	122.1 (9)

N4—C4—H4	118.2	N5—C14—H14	119.0
C17—C18—C21	124.5 (8)	N3A—C3A—Au2A	174.7
C19—C18—C21	120.2 (9)	C3A—Au2A—Au1	88.63 (19)
C19—C18—C17	115.4 (9)	C2A—Au2A—Au1	101.1 (2)
C8—N4—Fe1	121.6 (5)	C2A—Au2A—C3A	169.8
C4—N4—Fe1	120.0 (5)	N2A—C2A—Au2A	178.6
C4—N4—C8	117.1 (7)	N3B—C3B—Au2B	179.57 (10)
C18—C21—H21	117.8	C3B—Au2B—Au1	89.4 (6)
C21 ⁱⁱⁱ —C21—C18	124.4 (12)	C2B—Au2B—Au1	105.7 (7)
C21 ⁱⁱⁱ —C21—H21	117.8	C2B—Au2B—C3B	156.3
C6—C9—H9	116.6	N2B—C2B—Au2B	174.6
C10—C9—H9	116.6	H2A—O2—H2B	110.8
C10—C9—C6	126.9 (8)	H3B—O3—H3A	104.8
C18—C17—H17	120.4	H3A—O3—H3C	120.1
C18—C17—C16	119.2 (9)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O2	0.93	1.86	2.744 (13)	156
O1—H1B \cdots N6	0.93	1.85	2.736 (9)	158
C7—H7 \cdots N2B	0.93	2.08	2.78 (3)	132
N5—H5A \cdots N5 ^{iv}	0.86	1.82	2.677 (14)	176
O2—H2A \cdots N2A ⁱⁱ	0.96	2.49	3.45 (7)	179
O2—H2B \cdots N3B ^v	0.94	2.43	3.37 (3)	172
O3—H3B \cdots N3A	0.92	2.08	2.99 (3)	167
O3—H3A \cdots N2A ^{vi}	0.92	2.11	2.98 (4)	159
O3—H3C \cdots O3 ^{vii}	0.94	1.75	2.69 (4)	179

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