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catena-Poly[[diaquabis[1,4-bis(pyridin-4-yl)buta-1,3-diyne-κN]iron(II)]-μ-cyanido-$\kappa^2 N$:C-[dicyanido-$\kappa^2 C$-platinum(II)]-μ-cyanido-$\kappa^2 C$:N]

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Keywords: crystal structure; bitopic bpb ligand; hydrogen bonding; π–π stacking interactions.

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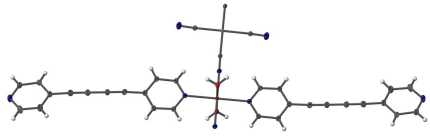
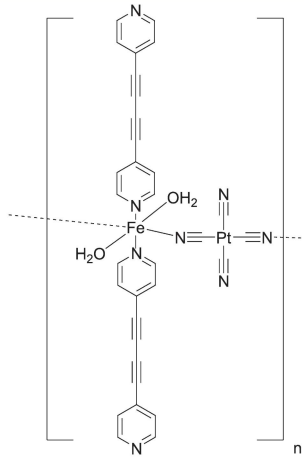
The molecular structure of the title compound, $[FePt(CN)_4(C_{14}H_8N_2)_2(H_2O)_2]_n$, consists of one-dimensional polymeric $[–Fe–NC–Pt(CN)_2–CN–]_\infty$ chains. Two water molecules and two monodentate 1,4-bis(pyridin-4-yl)buta-1,3-diyne (bpb) ligand molecules complete the octahedral coordination sphere of the Fe^{II} atoms. The Fe—N(py) bond length (py is pyridine) is 2.2700 (15) Å, Fe—N(cyanide) is 2.1185 (16) Å and the Fe—O distance is 2.1275 (14) Å. The water molecules are hydrogen bonded to either bpb ligands or cyanide groups of the planar $[Pt(CN)_4]^{2-}$ anion of adjacent polymeric chains. These O—H···N hydrogen bonds, in conjunction with offset and tilted π–π stacking interactions between bpb ligands and cyanide groups, extend the one-dimensional chains into a three-dimensional assembly.

3D view



Chemical scheme



Structure description

The title compound $[Fe(bpb)_2(H_2O)_2\{Pt(CN)_4\}_n$ (bpb = bis(pyridin-4-yl)butadiyne) results from ongoing research concerning the synthesis of Fe^{II} spin-crossover metal–organic frameworks containing polycyanometallates (Piñeiro-López *et al.*, 2014, 2017). The title compound was obtained as a side product during the synthesis of Hofmann clathrate $[Fe(bpb)_2[Pt(CN)_4]$·guest (Piñeiro-López *et al.*, 2014). The structure of the compound is similar to that of a one-dimensional linear polymer with a bridging $[Au(CN)_2]^-$-anion and a bitopic pyrazole-based ligand, $\{FeL_2(H_2O)_2[Au(CN)_2]\}_n$ (L = bis(3,5-dimethyl-1*H*-pyrazolyl)selenide)(Seredyuk *et al.*, 2007). Major structural differ-

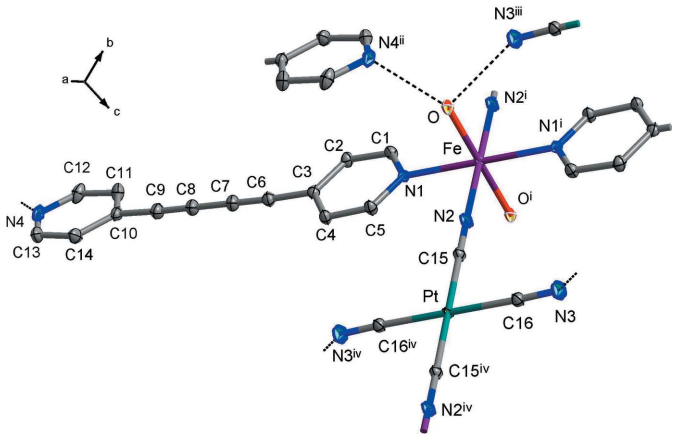


Figure 1
A fragment of the structure of the title compound showing hydrogen bonds with adjacent polymeric chains (dashed lines). [Symmetry codes: (i) $-x, 1-y, -z$; (ii) $2-x, -y, -1-z$; (iii) $-x, 1-y, -z$; (iv): $-x, -y, -z$.]

ences are attributed to the linear $[Au(CN)_2]^-$-bridging units instead of $[Pt(CN)_4]^{2-}$-anions, and a bent ligand *L*.

The molecular structure of the title compound $[Fe(bpb)_2(H_2O)_2\{Pt(CN)_4\}]_n$ (bpb = bis(pyridin-4-yl)butadiyne) consists of one-dimensional polymeric $[-Fe-NC-Pt(CN)_2-CN-]_\infty$ chains, repeating endlessly along [110] (Fig. 1). The Fe^{II} site has sixfold coordination with a distorted octahedral geometry, while the Pt^{II} ion is coordinated by four cyanide groups in an almost regular square-planar geometry. The metal ions reside on inversion centres. Two bitopic ligand molecules of bpb coordinate in a monodentate manner through a pyridine group together with two molecules of water and complete the octahedral coordination sphere of the Fe^{II} atoms. The Fe—N(py) bond length is 2.2700 (15) Å, $Fe-N_{(cyanide)}$ is 2.1185 (16) Å and the Fe—O distance is 2.1275 (14) Å. The second pyridine group of the ligand molecule and two cyano-groups of planar $[Pt(CN)_4]^{2-}$-anion form O—H···N hydrogen bonds (Table 1) with the water molecule belonging to adjacent polymeric chains. As a result of the hydrogen bonding, the dimensionality of the system is extended to a three-dimensional network (Fig. 2). A centroid-to-centroid distance of 3.6254 (10) Å between the pyridine rings of adjacent ligand molecules points to weak π–π stacking interactions.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H2*O*···N4^{i}	0.84 (3)	1.95 (3)	2.792 (2)	173 (3)
O—H1*O*···N3^{ii}	0.83 (3)	1.93 (3)	2.754 (2)	176 (3)

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

Synthesis and crystallization

Single crystals of the title compound were grown using the slow-diffusion technique. One side of a multi-arm-shaped vessel contained $(NH_4)_2Fe(SO_4)_2{\cdot}6H_2O$ (20 mg, 51 mmol) dissolved in water (0.5 ml). The contiguous arm contained solid bpb (11 mg, 49 mmol) and naphthalene (50 mg), and the third arm contained $K_2Pt(CN)_4{\cdot}3H_2O$ (22 mg, 51 mmol) in water (0.5 ml). The vessel was filled with a water/methanol (1:1) solution. Square-shaped light-red crystals suitable for single-crystal X-ray analysis were obtained in the middle arm after six weeks as a side product of the yellow-colored complex {Fe(pbp)[Pt(CN)$_4$]}.2naphthalene (Piñeiro-López *et al.*, 2014).

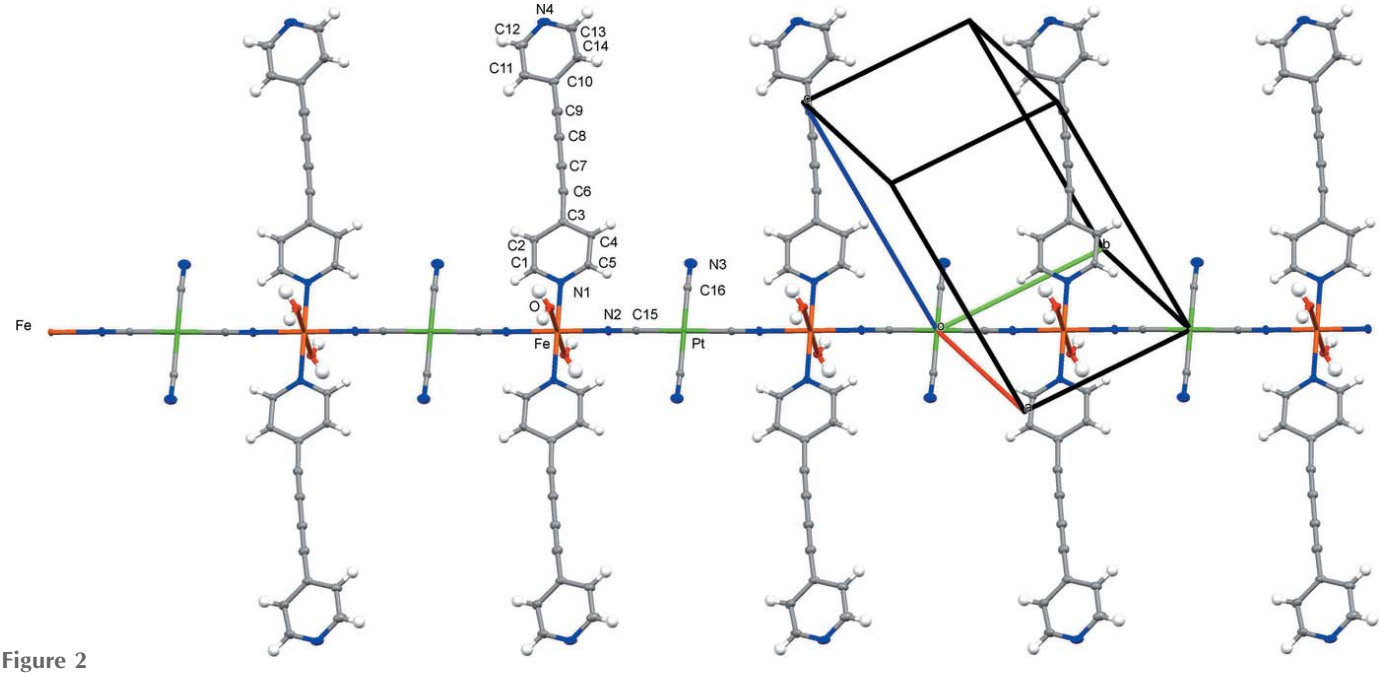


Figure 2
A fragment of the endless polymeric chain of the title compound with the atom-numbering scheme.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[FePt(CN)_4(C_{14}H_8N_2)_2(H_2O)_2]$
M_r	799.50
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	120
a, b, c (Å)	7.6572 (3), 9.0142 (4), 12.1781 (5)
α, β, γ (°)	106.975 (4), 102.042 (4), 102.408 (4)
V (Å^3)	751.31 (6)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.18
Crystal size (mm)	0.20 × 0.20 × 0.10
Data collection	
Diffractometer	Agilent SuperNova Sapphire3 CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min}, T_{max}	0.742, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14516, 4981, 4976
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.756
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.042, 1.02
No. of reflections	4981
No. of parameters	210
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.25, −1.16

Computer programs: *CrysAlis PRO* (Agilent, 2011), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg *et al.*, 1999) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
Brandenburg, K., Putz, H., or Brandenburg, K. & Berndt, M. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Piñeiro-López, L., Seredyuk, M., Muñoz, M. C. & Real, J. A. (2014). *Chem. Commun.* **50**, 1833–1835.
Piñeiro-López, L., Valverde-Muñoz, F. J., Seredyuk, M., Muñoz, M. C., Haukka, M. & Real, J. A. (2017). *Inorg. Chem.* **56**, 7038–7047.
Seredyuk, M., Haukka, M., Fritsky, I. O., Kozłowski, H., Krämer, R., Pavlenko, V. A. & Gütlich, P. (2007). *Dalton Trans.* pp. 3183–3194.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2017). **2**, x171413 [https://doi.org/10.1107/S2414314617014134]

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Crystal data

$[FePt(CN)_4(C_{14}H_8N_2)_2(H_2O)_2]$
M_r = 799.50
Triclinic, $P\overline{1}$
a = 7.6572 (3) Å
b = 9.0142 (4) Å
c = 12.1781 (5) Å
α = 106.975 (4)°
β = 102.042 (4)°
γ = 102.408 (4)°
V = 751.31 (6) Å^3
Z = 1
$F(000)$ = 388
D_x = 1.767 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 10158 reflections
θ = 3.2–32.4°
μ = 5.18 mm^{-1}
T = 120 K
Prismatic, red
0.20 × 0.20 × 0.10 mm

Data collection

Agilent SuperNova Sapphire3 CCD diffractometer
ω and phi scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2011)
T_{min} = 0.742, T_{max} = 1.000
14516 measured reflections
4981 independent reflections
4976 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 32.5°, θ_{min} = 3.2°
h = −11→11
k = −13→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.042
S = 1.02
4981 reflections
210 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0162P)^2 + 0.1718P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

Special details

Experimental. CrysAlisPro (Agilent Technologies, 2011). Version 1.171.36.21 (release 14-08-2012 CrysAlis171 .NET) (compiled Sep 14 2012,17:21:16) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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.

Refinement. H atoms attached to carbon atoms were positioned geometrically and constrained to ride on their parent atoms, with carbon hydrogen bond distances of 0.93. U_{iso}(H) values were set to 1.2 times U_{eq}(C). Water H atoms were freely refined with isotropic displacment parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt	0.0000	0.0000	0.0000	0.00881 (3)
Fe	0.5000	0.5000	0.0000	0.00981 (6)
O	0.33280 (19)	0.50060 (16)	−0.16295 (12)	0.0145 (2)
N1	0.6289 (2)	0.32518 (18)	−0.10666 (13)	0.0124 (3)
N2	0.2964 (2)	0.29769 (19)	−0.00226 (15)	0.0152 (3)
N3	−0.1740 (3)	0.2499 (2)	0.14476 (16)	0.0240 (4)
N4	1.4798 (3)	−0.4687 (2)	−0.66180 (15)	0.0215 (3)
C1	0.7935 (3)	0.3832 (2)	−0.12515 (16)	0.0137 (3)
H1	0.8500	0.4948	−0.0940	0.016*
C2	0.8827 (3)	0.2854 (2)	−0.18806 (16)	0.0148 (3)
H2	0.9958	0.3310	−0.1991	0.018*
C3	0.8008 (3)	0.1176 (2)	−0.23471 (15)	0.0142 (3)
C4	0.6312 (3)	0.0555 (2)	−0.21480 (16)	0.0157 (3)
H4	0.5730	−0.0557	−0.2435	0.019*
C5	0.5516 (3)	0.1633 (2)	−0.15140 (16)	0.0148 (3)
H5	0.4383	0.1211	−0.1392	0.018*
C6	0.8927 (3)	0.0153 (2)	−0.29969 (16)	0.0169 (3)
C7	0.9788 (3)	−0.0622 (2)	−0.35286 (17)	0.0183 (4)
C8	1.0789 (3)	−0.1493 (2)	−0.41274 (17)	0.0189 (4)
C9	1.1658 (3)	−0.2256 (3)	−0.46534 (18)	0.0202 (4)
C10	1.2732 (3)	−0.3111 (2)	−0.52906 (16)	0.0170 (3)
C11	1.4542 (3)	−0.2291 (3)	−0.52251 (17)	0.0209 (4)
H11	1.5088	−0.1207	−0.4736	0.025*
C12	1.5506 (3)	−0.3122 (3)	−0.59017 (17)	0.0234 (4)
H12	1.6707	−0.2567	−0.5857	0.028*
C13	1.3085 (3)	−0.5469 (2)	−0.66547 (18)	0.0218 (4)
H13	1.2591	−0.6561	−0.7135	0.026*
C14	1.1998 (3)	−0.4747 (2)	−0.60171 (18)	0.0209 (4)
H14	1.0808	−0.5339	−0.6073	0.025*
C15	0.1904 (3)	0.1867 (2)	−0.00073 (16)	0.0124 (3)
C16	−0.1121 (3)	0.1558 (2)	0.09247 (16)	0.0140 (3)
H1O	0.280 (4)	0.572 (3)	−0.158 (2)	0.027 (7)*
H2O	0.390 (4)	0.499 (3)	−0.215 (2)	0.032 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt	0.00875 (5)	0.00567 (4)	0.01247 (4)	0.00113 (3)	0.00495 (3)	0.00329 (3)
Fe	0.00918 (16)	0.00634 (14)	0.01392 (15)	0.00104 (12)	0.00582 (12)	0.00276 (12)
O	0.0158 (6)	0.0138 (6)	0.0161 (6)	0.0074 (5)	0.0074 (5)	0.0043 (5)
N1	0.0133 (7)	0.0104 (7)	0.0136 (6)	0.0033 (6)	0.0054 (5)	0.0034 (5)
N2	0.0147 (7)	0.0102 (7)	0.0222 (7)	0.0033 (6)	0.0093 (6)	0.0052 (6)
N3	0.0276 (10)	0.0241 (9)	0.0242 (8)	0.0155 (8)	0.0101 (7)	0.0069 (7)
N4	0.0253 (9)	0.0269 (9)	0.0163 (7)	0.0152 (8)	0.0091 (7)	0.0057 (6)
C1	0.0132 (8)	0.0112 (7)	0.0161 (7)	0.0036 (6)	0.0047 (6)	0.0035 (6)
C2	0.0131 (8)	0.0153 (8)	0.0162 (7)	0.0051 (7)	0.0057 (6)	0.0045 (6)
C3	0.0162 (8)	0.0157 (8)	0.0113 (7)	0.0072 (7)	0.0037 (6)	0.0041 (6)
C4	0.0178 (9)	0.0112 (8)	0.0166 (8)	0.0040 (7)	0.0067 (7)	0.0016 (6)
C5	0.0140 (8)	0.0121 (8)	0.0177 (8)	0.0032 (7)	0.0074 (7)	0.0030 (6)
C6	0.0187 (9)	0.0155 (8)	0.0158 (8)	0.0061 (7)	0.0051 (7)	0.0039 (6)
C7	0.0213 (10)	0.0179 (9)	0.0169 (8)	0.0079 (8)	0.0079 (7)	0.0046 (7)
C8	0.0219 (10)	0.0188 (9)	0.0181 (8)	0.0082 (8)	0.0084 (7)	0.0059 (7)
C9	0.0236 (10)	0.0211 (9)	0.0187 (8)	0.0094 (8)	0.0089 (8)	0.0072 (7)
C10	0.0222 (10)	0.0190 (9)	0.0137 (7)	0.0107 (8)	0.0082 (7)	0.0062 (6)
C11	0.0217 (10)	0.0210 (9)	0.0159 (8)	0.0065 (8)	0.0055 (7)	0.0004 (7)
C12	0.0183 (10)	0.0331 (11)	0.0168 (8)	0.0094 (9)	0.0063 (7)	0.0039 (8)
C13	0.0317 (11)	0.0174 (9)	0.0204 (9)	0.0116 (8)	0.0133 (8)	0.0055 (7)
C14	0.0266 (10)	0.0183 (9)	0.0241 (9)	0.0096 (8)	0.0152 (8)	0.0087 (7)
C15	0.0132 (8)	0.0104 (7)	0.0148 (7)	0.0047 (6)	0.0061 (6)	0.0037 (6)
C16	0.0139 (8)	0.0120 (8)	0.0165 (8)	0.0037 (7)	0.0059 (6)	0.0045 (6)

Geometric parameters (Å, º)

Pt—C15^{i}	1.9790 (17)	C2—C3	1.395 (3)
Pt—C15	1.9790 (17)	C2—H2	0.9300
Pt—C16	1.9940 (18)	C3—C4	1.398 (2)
Pt—C16^{i}	1.9941 (18)	C3—C6	1.434 (2)
Fe—N2^{ii}	2.1185 (16)	C4—C5	1.387 (2)
Fe—N2	2.1186 (16)	C4—H4	0.9300
Fe—O^{ii}	2.1275 (14)	C5—H5	0.9300
Fe—O	2.1275 (14)	C6—C7	1.206 (3)
Fe—N1	2.2700 (15)	C7—C8	1.376 (3)
Fe—N1^{ii}	2.2700 (15)	C8—C9	1.202 (3)
O—H1O	0.83 (3)	C9—C10	1.435 (3)
O—H2O	0.84 (3)	C10—C14	1.395 (3)
N1—C5	1.344 (2)	C10—C11	1.397 (3)
N1—C1	1.348 (2)	C11—C12	1.384 (3)
N2—C15	1.153 (3)	C11—H11	0.9300
N3—C16	1.154 (2)	C12—H12	0.9300
N4—C13	1.334 (3)	C13—C14	1.388 (3)
N4—C12	1.341 (3)	C13—H13	0.9300
C1—C2	1.383 (2)	C14—H14	0.9300

C1—H1	0.9300

C15^{i}—Pt—C15	180.0	C1—C2—H2	120.4
C15^{i}—Pt—C16	91.15 (7)	C3—C2—H2	120.4
C15—Pt—C16	88.85 (7)	C2—C3—C4	118.07 (16)
C15^{i}—Pt—C16^{i}	88.85 (7)	C2—C3—C6	119.49 (16)
C15—Pt—C16^{i}	91.15 (7)	C4—C3—C6	122.43 (17)
C16—Pt—C16^{i}	180.0	C5—C4—C3	118.65 (16)
N2^{ii}—Fe—N2	180.0	C5—C4—H4	120.7
N2^{ii}—Fe—O^{ii}	92.14 (6)	C3—C4—H4	120.7
N2—Fe—O^{ii}	87.86 (6)	N1—C5—C4	123.74 (16)
N2^{ii}—Fe—O	87.86 (6)	N1—C5—H5	118.1
N2—Fe—O	92.14 (6)	C4—C5—H5	118.1
O^{ii}—Fe—O	180.0	C7—C6—C3	175.9 (2)
N2^{ii}—Fe—N1	91.29 (6)	C6—C7—C8	179.3 (2)
N2—Fe—N1	88.71 (6)	C9—C8—C7	179.8 (3)
O^{ii}—Fe—N1	90.25 (5)	C8—C9—C10	177.7 (2)
O—Fe—N1	89.75 (5)	C14—C10—C11	118.15 (17)
N2^{ii}—Fe—N1^{ii}	88.71 (6)	C14—C10—C9	121.82 (18)
N2—Fe—N1^{ii}	91.29 (6)	C11—C10—C9	119.99 (18)
O^{ii}—Fe—N1^{ii}	89.75 (5)	C12—C11—C10	118.77 (19)
O—Fe—N1^{ii}	90.25 (5)	C12—C11—H11	120.6
N1—Fe—N1^{ii}	180.0	C10—C11—H11	120.6
Fe—O—H1O	117.1 (18)	N4—C12—C11	123.4 (2)
Fe—O—H2O	112.8 (19)	N4—C12—H12	118.3
H1O—O—H2O	109 (3)	C11—C12—H12	118.3
C5—N1—C1	116.97 (15)	N4—C13—C14	123.71 (19)
C5—N1—Fe	123.42 (11)	N4—C13—H13	118.1
C1—N1—Fe	119.59 (11)	C14—C13—H13	118.1
C15—N2—Fe	177.61 (18)	C13—C14—C10	118.53 (19)
C13—N4—C12	117.42 (17)	C13—C14—H14	120.7
N1—C1—C2	123.43 (16)	C10—C14—H14	120.7
N1—C1—H1	118.3	N2—C15—Pt	177.63 (18)
C2—C1—H1	118.3	N3—C16—Pt	177.73 (17)
C1—C2—C3	119.12 (16)		

C5—N1—C1—C2	0.8 (3)	C3—C4—C5—N1	−0.6 (3)
Fe—N1—C1—C2	179.39 (13)	C14—C10—C11—C12	1.5 (3)
N1—C1—C2—C3	−0.5 (3)	C9—C10—C11—C12	−176.41 (19)
C1—C2—C3—C4	−0.4 (3)	C13—N4—C12—C11	−1.1 (3)
C1—C2—C3—C6	−179.78 (17)	C10—C11—C12—N4	−0.4 (3)
C2—C3—C4—C5	0.9 (3)	C12—N4—C13—C14	1.4 (3)
C6—C3—C4—C5	−179.76 (17)	N4—C13—C14—C10	−0.3 (3)
C1—N1—C5—C4	−0.3 (3)	C11—C10—C14—C13	−1.2 (3)
Fe—N1—C5—C4	−178.80 (14)	C9—C10—C14—C13	176.68 (19)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H2*O*···N4^{iii}	0.84 (3)	1.95 (3)	2.792 (2)	173 (3)
O—H1*O*···N3^{iv}	0.83 (3)	1.93 (3)	2.754 (2)	176 (3)

Symmetry codes: (iii) −*x*+2, −*y*, −*z*−1; (iv) −*x*, −*y*+1, −*z*.