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Diaquabis{5-(pyridin-2-yl-κN)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-1-ido-κN^1}iron(II)

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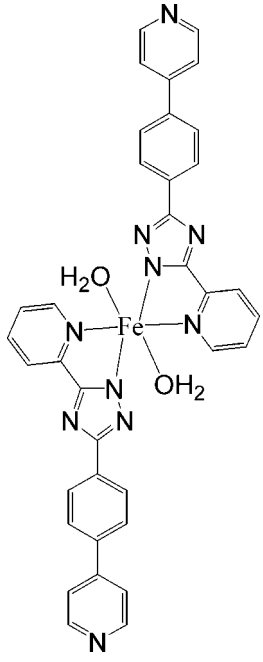
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.059; wR factor = 0.184; data-to-parameter ratio = 11.8.

In the centrosymmetric title complex, $[Fe(C_{18}H_{12}N_5)_2(H_2O)_2]$, the Fe^{II} ion, lying on an inversion centre, is coordinated by two *N*,*N*′-bidentate 5-(pyridin-2-yl)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-1-ide ligands and two water molecules in a *trans*-FeO_2N_4 geometry. In the ligand, the triazole ring makes dihedral angles of 5.21 (18) and 6.7 (2)°, respectively, with the adjacent pyridine and benzene rings. In the crystal, molecules are linked by O—H···N hydrogen bonds, generating a three-dimensional network.

Related literature

For background to coordination complexes, see: Zhang, Sun *et al.* (2012); Zhang, Fan *et al.* (2012); Fan *et al.* (2013).



Experimental

Crystal data

$[Fe(C_{18}H_{12}N_5)_2(H_2O)_2]$
M_r = 688.53
Monoclinic, $P2_1/c$
a = 13.1965 (17) Å
b = 12.0279 (16) Å
c = 9.9006 (13) Å
β = 100.998 (1)°
V = 1542.6 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 296 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.938, T_{max} = 0.958
7711 measured reflections
2722 independent reflections
2214 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.184
S = 1.00
2722 reflections
231 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*W*···N4^{i}	0.81 (4)	1.99 (4)	2.784 (4)	168 (4)
O1—H2*W*···N5^{ii}	0.85 (5)	2.39 (5)	3.165 (6)	152 (5)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5245).

References

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Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Zhang, X.-T., Fan, L.-M., Zhao, X., Sun, D., Li, D.-C. & Dou, J.-M. (2012). *CrystEngComm*, **14**, 2053–2061.
Zhang, X.-T., Sun, D., Li, B., Fan, L.-M., Li, B. & Wei, P.-H. (2012). *Cryst. Growth Des.* **12**, 3845–3848.

supporting information

Acta Cryst. (2013). E**69**, m168 [doi:10.1107/S1600536813004601]

Diaquabis{5-(pyridin-2-yl-κN)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-1-ido-κN^1}iron(II)

Bin Li

S1. Comment

The design and synthesis of coordination complexes have attracted upsurging research interest not only because of their appealing structural and topological novelty but also owing to their tremendous potential applications in gas storage, microelectronics, ion exchange, chemical separations, nonlinear optics and heterogeneous catalysis (Zhang, Sun *et al.*, 2012; Zhang, Fan *et al.*, 2012; Fan *et al.*, 2013). Here, we report one new compound, $[Fe(H_2O)_2(C_{18}H_{12}N_5)_2]$, obtained from the solvothermal reaction of 2-{3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-5-yl}pyridine and iron(II) chloride tetrahydrate.

The asymmetric unit of the title compound consists of a half of Fe(II), one deprotonated 2-{3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-5-}pyridine, and one water molecule. The Fe atom owns a distorted octahedral coordination geometry, completed by four N atoms from two deprotonated 2-{3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-5-yl}pyridine and two O atoms from two water molecules (Fig. 1). The Fe—O distance is 2.205 (3) Å. The Fe—N distances are 2.103 (3) and 2.171 (3) Å. The O—H···N hydrogen bonds (Table 1) in the crystal lead to a consolidation of the structure (Fig. 2) .

S2. Experimental

A mixture of 2-{3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-5-yl}pyridine (0.20 mmol, 0.060 g), iron(II) chloride tetrahydrate (0.40 mmol, 0.078 g), NaOH (0.20 mmol, 0.008 g) and 12 mL H_2O was placed in a Teflon-lined stainless steel vessel, heated to 170 °C for 3 days, followed by slow cooling (a descent rate of 10 °C/h) to room temperature. Red crystals suitable for the X-ray experiment were obtained. Anal. Calc. for $C_{36}H_{28}FeN_{10}O_2$: C 62.80, H 4.10, N 20.34%; Found: C 62.72, H 4.03, N 20.18%.

S3. Refinement

All H atoms bound to C were refined using a riding model with C—H = 0.93 Å, and with $U_{iso} = 1.2U_{eq}$ (C). The H atoms of the water molecule were located in a difference Fourier map and were refined with distance restraints of O—H = 0.820 (1) and H···H = 1.380 (1) Å [O—H = 0.81 (4) and 0.85 (5) Å].

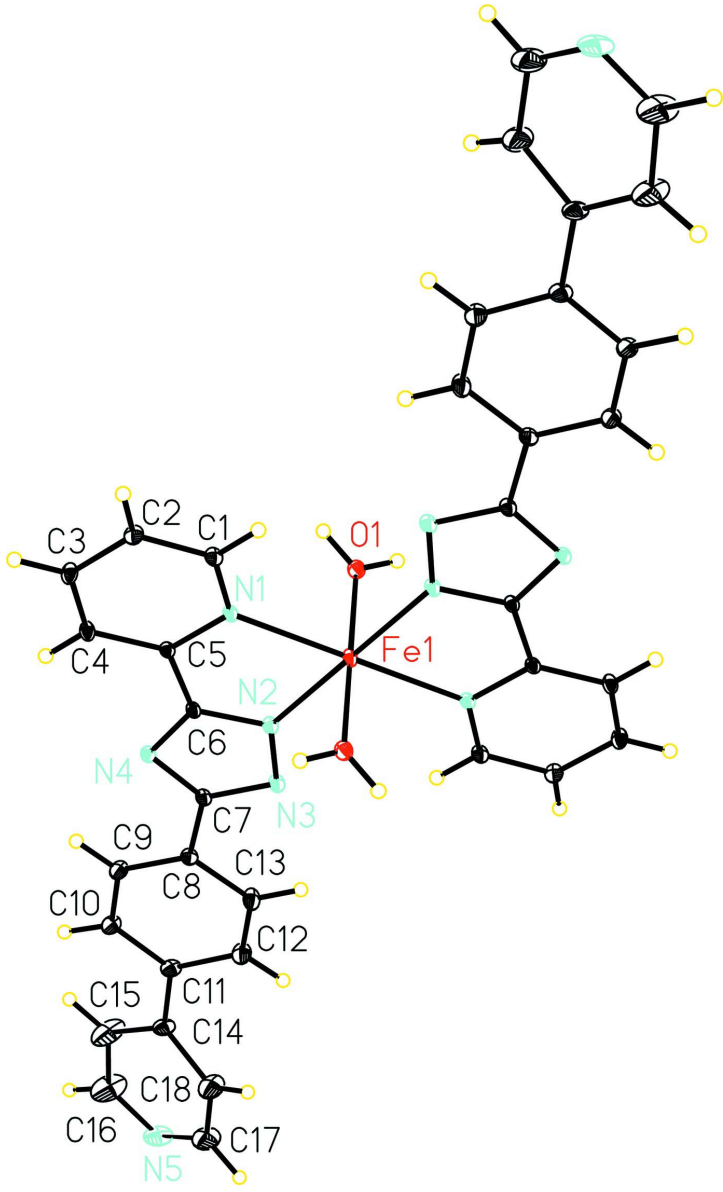

Figure 1

The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are given as spheres of arbitrary radius.

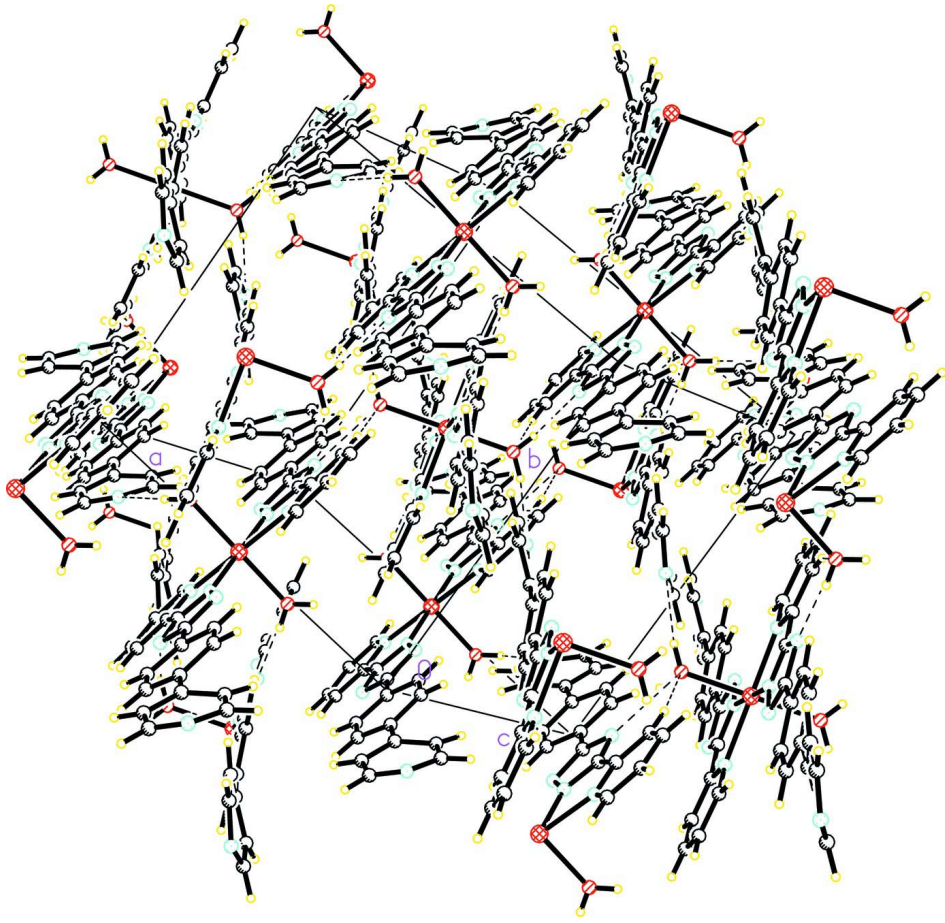

Figure 2

A crystal packing view of the title compound, displayed with hydrogen bonds as dashed lines.

Diaquabis{5-(pyridin-2-yl-*κN*)-3-[4-(pyridin-4-yl)phenyl]-1*H*-1,2,4-triazol-1-ido-*κN*^{1}}iron(II)

Crystal data

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c = 9.9006 (13) Å
β = 100.998 (1)°
V = 1542.6 (4) Å^3
Z = 2
$F(000)$ = 712
D_x = 1.482 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 425 reflections
θ = 2.3–16.0°
μ = 0.54 mm^{-1}
T = 296 K
Block, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.938, T_{max} = 0.958
7711 measured reflections
2722 independent reflections
2214 reflections with $I > 2\sigma(I)$

R_{int} = 0.035
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −11→15
k = −13→14
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.184
S = 1.00
2722 reflections
231 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.120P)^2 + 1.3369P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.3747 (3)	0.2112 (3)	−0.1244 (4)	0.0363 (8)
H1	0.3428	0.1627	−0.1925	0.044*
C2	0.3486 (3)	0.3216 (3)	−0.1351 (4)	0.0412 (9)
H2	0.3004	0.3476	−0.2095	0.049*
C3	0.3951 (3)	0.3931 (3)	−0.0334 (4)	0.0425 (9)
H3	0.3786	0.4683	−0.0383	0.051*
C4	0.4663 (3)	0.3527 (3)	0.0757 (4)	0.0377 (9)
H4	0.4977	0.4000	0.1455	0.045*
C5	0.4900 (2)	0.2410 (3)	0.0795 (3)	0.0285 (7)
C6	0.5674 (2)	0.1872 (3)	0.1860 (3)	0.0280 (7)
C7	0.6842 (3)	0.1449 (3)	0.3520 (3)	0.0310 (8)
C8	0.7662 (3)	0.1451 (3)	0.4768 (3)	0.0357 (8)
C9	0.7863 (3)	0.2334 (4)	0.5670 (4)	0.0468 (10)
H9	0.7465	0.2976	0.5507	0.056*
C10	0.8648 (3)	0.2276 (4)	0.6809 (4)	0.0512 (11)
H10	0.8764	0.2881	0.7403	0.061*
C11	0.9267 (3)	0.1348 (4)	0.7094 (4)	0.0456 (10)
C12	0.9037 (4)	0.0443 (4)	0.6214 (5)	0.0576 (12)
H12	0.9421	−0.0207	0.6395	0.069*
C13	0.8253 (4)	0.0489 (3)	0.5086 (5)	0.0557 (12)
H13	0.8112	−0.0132	0.4522	0.067*

C14	1.0144 (3)	0.1269 (4)	0.8279 (4)	0.0515 (11)
C15	1.0280 (5)	0.1932 (7)	0.9391 (6)	0.124 (3)
H15	0.9809	0.2496	0.9455	0.149*
C16	1.1133 (6)	0.1770 (8)	1.0451 (6)	0.132 (4)
H16	1.1206	0.2259	1.1191	0.158*
C17	1.1777 (5)	0.0489 (6)	0.9320 (7)	0.0927 (19)
H17	1.2319	0.0018	0.9229	0.111*
C18	1.0973 (5)	0.0595 (6)	0.8208 (6)	0.0885 (19)
H18	1.0993	0.0205	0.7403	0.106*
Fe1	0.5000	0.0000	0.0000	0.0319 (3)
N1	0.4444 (2)	0.1702 (2)	−0.0198 (3)	0.0300 (6)
N2	0.5878 (2)	0.0804 (2)	0.1719 (3)	0.0335 (7)
N3	0.6647 (2)	0.0523 (2)	0.2789 (3)	0.0371 (7)
N4	0.6261 (2)	0.2328 (2)	0.2991 (3)	0.0307 (7)
N5	1.1827 (3)	0.1012 (5)	1.0503 (4)	0.0787 (14)
O1	0.3849 (2)	−0.0453 (3)	0.1252 (3)	0.0406 (6)
H1W	0.374 (3)	−0.110 (4)	0.140 (5)	0.063 (15)*
H2W	0.336 (4)	−0.002 (3)	0.136 (5)	0.055 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.040 (2)	0.0363 (18)	0.0265 (18)	−0.0005 (16)	−0.0088 (15)	−0.0023 (15)
C2	0.044 (2)	0.038 (2)	0.034 (2)	0.0095 (17)	−0.0115 (16)	0.0047 (16)
C3	0.054 (2)	0.0281 (18)	0.040 (2)	0.0084 (17)	−0.0064 (17)	0.0031 (15)
C4	0.047 (2)	0.0277 (17)	0.0325 (19)	−0.0005 (15)	−0.0077 (16)	−0.0042 (15)
C5	0.0304 (17)	0.0278 (16)	0.0244 (17)	−0.0019 (13)	−0.0024 (13)	−0.0018 (13)
C6	0.0319 (17)	0.0238 (16)	0.0248 (17)	−0.0027 (13)	−0.0036 (13)	0.0009 (13)
C7	0.0350 (18)	0.0304 (17)	0.0234 (17)	−0.0018 (14)	−0.0046 (14)	−0.0003 (14)
C8	0.0352 (19)	0.0381 (19)	0.0283 (18)	0.0013 (15)	−0.0077 (14)	−0.0014 (15)
C9	0.044 (2)	0.051 (2)	0.038 (2)	0.0121 (18)	−0.0089 (17)	−0.0124 (18)
C10	0.044 (2)	0.063 (3)	0.039 (2)	0.012 (2)	−0.0115 (17)	−0.022 (2)
C11	0.038 (2)	0.064 (3)	0.0303 (19)	0.0060 (19)	−0.0057 (16)	−0.0057 (19)
C12	0.058 (3)	0.049 (2)	0.054 (3)	0.013 (2)	−0.020 (2)	0.000 (2)
C13	0.062 (3)	0.040 (2)	0.052 (3)	0.007 (2)	−0.023 (2)	−0.009 (2)
C14	0.036 (2)	0.075 (3)	0.038 (2)	0.008 (2)	−0.0067 (17)	−0.005 (2)
C15	0.088 (4)	0.196 (8)	0.064 (4)	0.067 (5)	−0.048 (3)	−0.063 (5)
C16	0.094 (5)	0.225 (10)	0.056 (4)	0.048 (6)	−0.038 (3)	−0.061 (5)
C17	0.063 (4)	0.120 (5)	0.080 (4)	0.018 (4)	−0.024 (3)	0.002 (4)
C18	0.071 (4)	0.107 (5)	0.072 (4)	0.028 (3)	−0.025 (3)	−0.016 (3)
Fe1	0.0380 (5)	0.0226 (4)	0.0274 (4)	0.0003 (3)	−0.0131 (3)	−0.0020 (3)
N1	0.0311 (15)	0.0258 (14)	0.0277 (14)	−0.0008 (11)	−0.0080 (11)	−0.0002 (11)
N2	0.0377 (16)	0.0274 (14)	0.0278 (15)	0.0006 (12)	−0.0127 (12)	0.0005 (12)
N3	0.0397 (17)	0.0308 (15)	0.0317 (16)	0.0013 (13)	−0.0158 (13)	−0.0009 (13)
N4	0.0320 (15)	0.0299 (14)	0.0260 (14)	0.0000 (12)	−0.0054 (12)	−0.0047 (12)
N5	0.050 (2)	0.130 (4)	0.045 (2)	0.010 (3)	−0.0188 (18)	0.004 (3)
O1	0.0414 (16)	0.0322 (15)	0.0438 (15)	0.0010 (13)	−0.0031 (12)	0.0047 (13)

Geometric parameters (Å, º)

C1—N1	1.341 (4)	C11—C12	1.391 (6)
C1—C2	1.371 (5)	C11—C14	1.485 (5)
C1—H1	0.9300	C12—C13	1.371 (6)
C2—C3	1.376 (5)	C12—H12	0.9300
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.378 (5)	C14—C15	1.344 (7)
C3—H3	0.9300	C14—C18	1.374 (7)
C4—C5	1.378 (5)	C15—C16	1.398 (7)
C4—H4	0.9300	C15—H15	0.9300
C5—N1	1.352 (4)	C16—N5	1.287 (9)
C5—C6	1.470 (4)	C16—H16	0.9300
C6—N2	1.325 (4)	C17—N5	1.320 (8)
C6—N4	1.350 (4)	C17—C18	1.381 (7)
C7—N3	1.327 (4)	C17—H17	0.9300
C7—N4	1.351 (4)	C18—H18	0.9300
C7—C8	1.479 (4)	Fe1—N2	2.103 (3)
C8—C9	1.380 (5)	Fe1—N1	2.171 (3)
C8—C13	1.397 (5)	Fe1—O1	2.205 (3)
C9—C10	1.380 (5)	N2—N3	1.363 (4)
C9—H9	0.9300	O1—H1W	0.81 (4)
C10—C11	1.381 (6)	O1—H2W	0.85 (5)
C10—H10	0.9300		

N1—C1—C2	122.8 (3)	C18—C14—C11	120.4 (4)
N1—C1—H1	118.6	C14—C15—C16	119.6 (6)
C2—C1—H1	118.6	C14—C15—H15	120.2
C1—C2—C3	118.5 (3)	C16—C15—H15	120.2
C1—C2—H2	120.7	N5—C16—C15	126.4 (6)
C3—C2—H2	120.7	N5—C16—H16	116.8
C2—C3—C4	119.7 (3)	C15—C16—H16	116.8
C2—C3—H3	120.1	N5—C17—C18	124.3 (6)
C4—C3—H3	120.1	N5—C17—H17	117.8
C5—C4—C3	118.9 (3)	C18—C17—H17	117.8
C5—C4—H4	120.6	C14—C18—C17	120.8 (6)
C3—C4—H4	120.6	C14—C18—H18	119.6
N1—C5—C4	121.8 (3)	C17—C18—H18	119.6
N1—C5—C6	113.3 (3)	N2—Fe1—N2^{i}	180.0 (2)
C4—C5—C6	124.9 (3)	N2—Fe1—N1^{i}	103.68 (10)
N2—C6—N4	112.6 (3)	N2^{i}—Fe1—N1^{i}	76.32 (10)
N2—C6—C5	118.6 (3)	N2—Fe1—N1	76.32 (10)
N4—C6—C5	128.8 (3)	N2^{i}—Fe1—N1	103.68 (10)
N3—C7—N4	114.1 (3)	N1^{i}—Fe1—N1	180.00 (14)
N3—C7—C8	119.4 (3)	N2—Fe1—O1^{i}	90.52 (11)
N4—C7—C8	126.4 (3)	N2^{i}—Fe1—O1^{i}	89.48 (11)
C9—C8—C13	117.5 (3)	N1^{i}—Fe1—O1^{i}	91.52 (11)
C9—C8—C7	124.1 (3)	N1—Fe1—O1^{i}	88.48 (11)

C13—C8—C7	118.4 (3)	N2—Fe1—O1	89.48 (11)
C10—C9—C8	120.7 (4)	N2^{i}—Fe1—O1	90.52 (11)
C10—C9—H9	119.6	N1^{i}—Fe1—O1	88.48 (11)
C8—C9—H9	119.6	N1—Fe1—O1	91.52 (11)
C9—C10—C11	122.1 (4)	O1^{i}—Fe1—O1	180.00 (19)
C9—C10—H10	119.0	C1—N1—C5	118.3 (3)
C11—C10—H10	119.0	C1—N1—Fe1	125.9 (2)
C10—C11—C12	117.0 (3)	C5—N1—Fe1	115.6 (2)
C10—C11—C14	123.7 (4)	C6—N2—N3	107.2 (3)
C12—C11—C14	119.3 (4)	C6—N2—Fe1	116.1 (2)
C13—C12—C11	121.3 (4)	N3—N2—Fe1	136.7 (2)
C13—C12—H12	119.4	C7—N3—N2	104.7 (3)
C11—C12—H12	119.4	C6—N4—C7	101.4 (3)
C12—C13—C8	121.3 (4)	C16—N5—C17	112.8 (5)
C12—C13—H13	119.4	Fe1—O1—H1W	121 (3)
C8—C13—H13	119.4	Fe1—O1—H2W	123 (3)
C15—C14—C18	114.1 (4)	H1W—O1—H2W	113 (4)
C15—C14—C11	124.8 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···N4^{ii}	0.81 (4)	1.99 (4)	2.784 (4)	168 (4)
O1—H2*W*···N5^{iii}	0.85 (5)	2.39 (5)	3.165 (6)	152 (5)

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