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(Methanolato)(pyridine)[N^2,$N^{2'}$-(pyridine-2,6-diyldicarbonyl)diacetohydrazide(2–)]iron(III) methanol solvate

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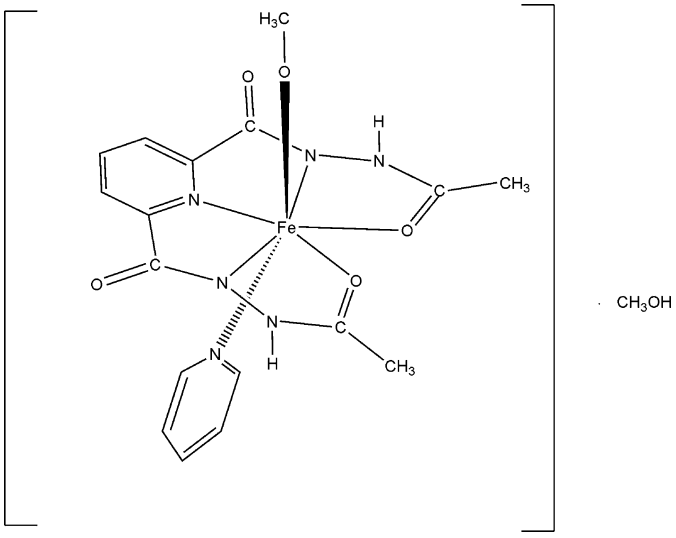
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.044; wR factor = 0.115; data-to-parameter ratio = 12.8.

In the title complex, $[Fe(C_{11}H_{10}N_5O_4)(CH_3O)(C_5H_5N)]\cdot CH_4O$, the Fe^{III} ion has a distorted pentagonal-bipyramidal geometry. In the crystal structure, molecules are linked into one-dimensional chains along $[1\bar{1}1]$ *via* intermolecular O—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Sreeja *et al.* (2004); Bonardi *et al.* (1991); Drozdzewski *et al.* (2006).



Experimental

Crystal data

$[Fe(C_{11}H_{10}N_5O_4)(CH_3O)(C_5H_5N)]\cdot CH_4O$
M_r = 475.27
Triclinic, $P\bar{1}$
a = 8.258 (10) Å
b = 10.64 (14) Å
c = 12.448 (18) Å
α = 83.518 (3)°
β = 85.924 (3)°
γ = 77.176 (2)°
V = 1058.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 298 (2) K
0.37 × 0.29 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.766, T_{max} = 0.863
5507 measured reflections
3658 independent reflections
2647 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.00
3658 reflections
285 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—O5	1.922 (3)	Fe1—O3	2.209 (2)
Fe1—N4	2.107 (3)	Fe1—N1	2.228 (3)
Fe1—O4	2.142 (2)	Fe1—N6	2.245 (3)
Fe1—N2	2.150 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.86	1.94	2.780 (3)	167
N5—H5···O6^{ii}	0.86	1.98	2.830 (4)	167
O6—H6···O5^{iii}	0.82	1.90	2.718 (3)	172

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

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2566).

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supporting information

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(Methanolato)(pyridine)[N^2,$N^{2'}$-(pyridine-2,6-diyldicarbonyl)-diacetohydrazide(2–)]iron(III) methanol solvate

Quan-Fu Cao, Jian-Min Dou, Da-Cheng Li and Da-Qi Wang

S1. Comment

Metal-hydrazide complexes, especially Fe complexes with acetylhydrazide, continue to attract considerable attention due to their biological activities and structural versatilities (Drozdzewski *et al.*, 2006; Sreeja *et al.*, 2004) We report herein, the crystal structure of the title complex. A view of the title complex (I) is shown in Fig.1. The Fe^{III} ion has a distorted pentagonal-bipyramidal coordination geometry, formed by one 2-oxido-N, N′-2,6-picoloylhydrazide ligand, one pyridine ligand and one methanol molecule. The distances involving atom Fe1 atom are consistent with those in a Fe complex with pentagonal-bipyramidal coordination geometry (Bonardi *et al.*, 1991). Both intermolecular O—H···O and N—H···O hydrogen bonding occur in the crystal structure (Table 2).

S2. Experimental

A pyridine solution (10 mL) of *N*,*N*′-diacetyl-2,6-picoloylhydrazide (0.2 mmol,0.0559 g) was mixed with a methanol solution (10 mL) of iron chloride (0.2 mmol, 0.0808 g). The mixture was stirred at room temperature for 6 h and then filtered. Dark block-shaped crystals of the title complex suitable for X-ray diffraction analysis were obtained after three weeks (m.p. >573 K). Elemental analysis calculated for $(C_{18}H_{23}N_6O_6)Fe$: C 45.49, H 4.88, N 17.68%; found: C 45.41, H 4.76, N 17.50%.

S3. Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms, with pyridine C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å, methanol hydroxyl O—H distances of 0.82 Å, hydrazide N—H distances of 0.86Å and U_{iso}(H)=1.2U_{eq}(C,*N*) or 1.5U_{eq}(O).

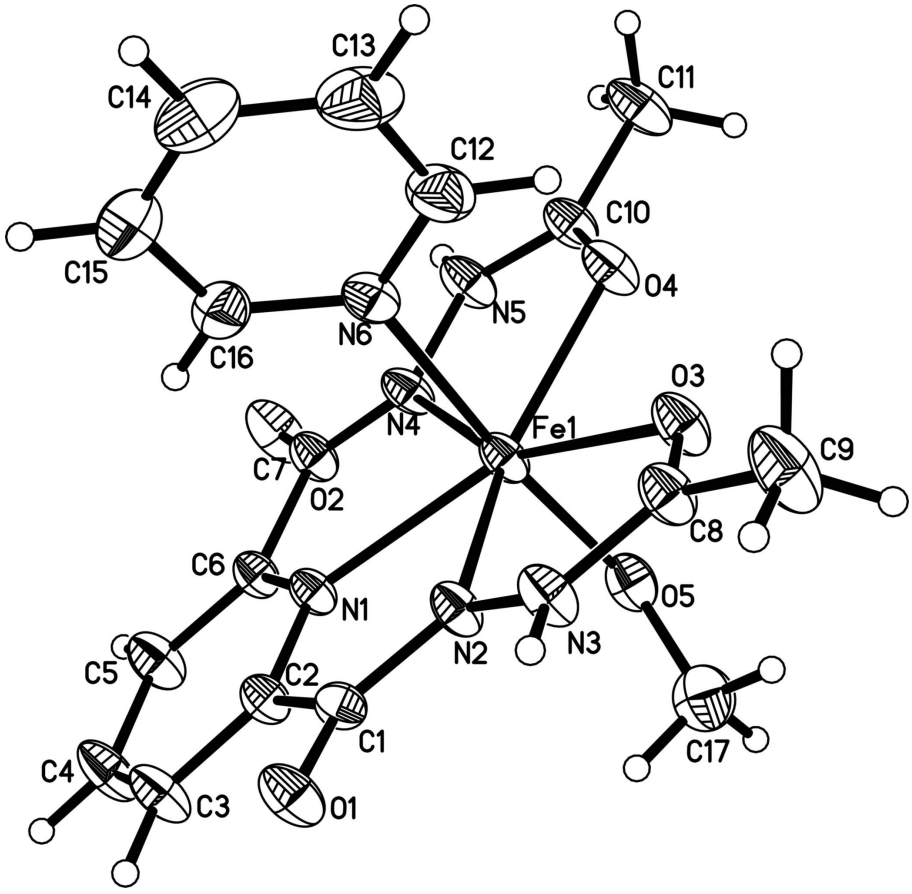

Figure 1

The molecular structure of the title complex. Displacement ellipsoids are drawn at 30% probability level and solvent molecule has been omitted for clarity.

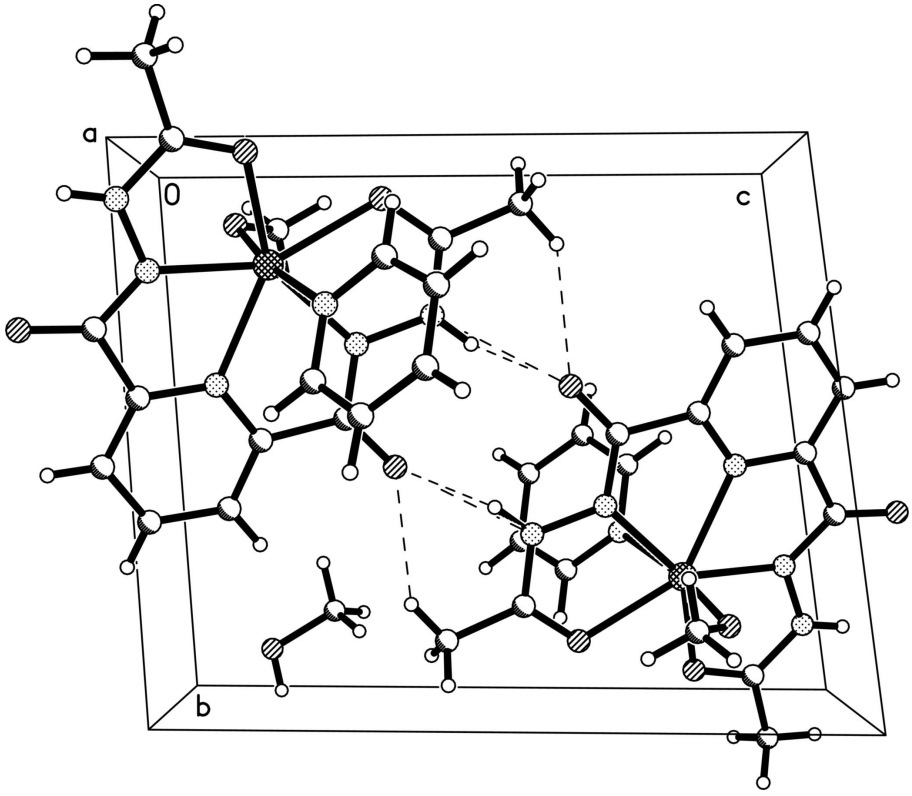

Figure 2

Part of the crystal structure with hydrogen bonds shown as dashed lines.

(Methanolato)(pyridine)[*N*^{2},*N*$^{2'}$-(pyridine-2,6- diyldicarbonyl)diacetohydrazide(2-)]iron(III) methanol solvate

Crystal data

$[Fe(C_{11}H_{10}N_5O_4)(CH_3O)(C_5H_5N)]\cdot CH_4O$
$M_r = 475.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.258$ (10) Å
$b = 10.64$ (14) Å
$c = 12.448$ (18) Å
$\alpha = 83.518$ (3)°
$\beta = 85.924$ (3)°
$\gamma = 77.176$ (2)°
$V = 1058.4$ (2) Å^3
$Z = 2$
$F(000) = 494$
$D_x = 1.491$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1856 reflections
$\theta = 2.4$–25.1°
$\mu = 0.76$ mm^{-1}
$T = 298$ K
Block, black
0.37 × 0.29 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.766$, $T_{max} = 0.863$
5507 measured reflections
3658 independent reflections
2647 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -9\rightarrow9$
$k = -12\rightarrow9$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.115$
$S = 1.00$
3658 reflections
285 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.050P)^2 + 0.8457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.31969 (6)	0.23928 (4)	0.23357 (4)	0.03344 (18)
N1	0.2243 (3)	0.4328 (2)	0.1451 (2)	0.0303 (6)
N2	0.1580 (4)	0.3649 (2)	0.3383 (2)	0.0338 (7)
N3	0.1451 (4)	0.3167 (3)	0.4458 (2)	0.0384 (7)
H3	0.0928	0.3633	0.4949	0.046*
N4	0.4403 (4)	0.2535 (3)	0.0791 (2)	0.0370 (7)
N5	0.5609 (4)	0.1455 (3)	0.0544 (2)	0.0423 (8)
H5	0.6117	0.1395	−0.0082	0.051*
N6	0.5139 (4)	0.3108 (3)	0.3122 (2)	0.0391 (7)
O1	0.0049 (3)	0.5677 (2)	0.37219 (18)	0.0445 (7)
O2	0.4513 (4)	0.3481 (2)	−0.0965 (2)	0.0585 (8)
O3	0.2966 (3)	0.1301 (2)	0.39371 (18)	0.0441 (7)
O4	0.5115 (3)	0.0678 (2)	0.22480 (18)	0.0427 (6)
O5	0.1500 (3)	0.1644 (2)	0.18472 (19)	0.0420 (6)
O6	0.7483 (4)	0.0858 (3)	0.8604 (2)	0.0673 (9)
H6	0.7754	0.0083	0.8528	0.101*
C1	0.0853 (4)	0.4869 (3)	0.3119 (3)	0.0309 (8)
C2	0.1142 (4)	0.5230 (3)	0.1937 (3)	0.0329 (8)
C3	0.0382 (5)	0.6368 (3)	0.1377 (3)	0.0466 (10)
H3A	−0.0392	0.6984	0.1725	0.056*
C4	0.0788 (5)	0.6583 (4)	0.0286 (3)	0.0543 (12)
H4	0.0276	0.7342	−0.0112	0.065*
C5	0.1959 (5)	0.5662 (3)	−0.0208 (3)	0.0473 (10)
H5A	0.2262	0.5796	−0.0939	0.057*
C6	0.2669 (4)	0.4542 (3)	0.0403 (3)	0.0331 (8)

C7	0.3972 (5)	0.3455 (3)	−0.0011 (3)	0.0374 (9)
C8	0.2196 (5)	0.1930 (3)	0.4677 (3)	0.0412 (9)
C9	0.2090 (6)	0.1342 (4)	0.5816 (3)	0.0655 (14)
H9A	0.1532	0.0636	0.5849	0.098*
H9B	0.1479	0.1984	0.6262	0.098*
H9C	0.3190	0.1026	0.6072	0.098*
C10	0.5907 (5)	0.0531 (3)	0.1351 (3)	0.0394 (9)
C11	0.7196 (5)	−0.0667 (4)	0.1174 (3)	0.0561 (12)
H11A	0.8101	−0.0731	0.1634	0.084*
H11B	0.7600	−0.0628	0.0431	0.084*
H11C	0.6714	−0.1413	0.1341	0.084*
C12	0.5929 (5)	0.2396 (4)	0.3965 (3)	0.0560 (11)
H12	0.5816	0.1544	0.4128	0.067*
C13	0.6902 (6)	0.2880 (6)	0.4597 (4)	0.0707 (14)
H13	0.7425	0.2363	0.5180	0.085*
C14	0.7092 (6)	0.4122 (6)	0.4364 (4)	0.0709 (14)
H14	0.7723	0.4472	0.4792	0.085*
C15	0.6335 (6)	0.4841 (5)	0.3486 (4)	0.0683 (13)
H15	0.6469	0.5684	0.3295	0.082*
C16	0.5374 (5)	0.4305 (4)	0.2890 (3)	0.0503 (10)
H16	0.4863	0.4804	0.2295	0.060*
C17	−0.0016 (6)	0.1640 (4)	0.2357 (4)	0.0607 (12)
H17A	0.0131	0.1184	0.3066	0.091*
H17B	−0.0639	0.1218	0.1945	0.091*
H17C	−0.0607	0.2516	0.2419	0.091*
C18	0.7218 (7)	0.1580 (4)	0.7573 (4)	0.0744 (15)
H18A	0.6765	0.2475	0.7668	0.112*
H18B	0.6454	0.1248	0.7195	0.112*
H18C	0.8257	0.1503	0.7160	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0429 (3)	0.0265 (3)	0.0255 (3)	0.0037 (2)	0.0005 (2)	−0.00328 (19)
N1	0.0369 (17)	0.0263 (14)	0.0241 (14)	0.0012 (12)	−0.0014 (12)	−0.0032 (11)
N2	0.0463 (18)	0.0276 (15)	0.0221 (14)	0.0017 (13)	0.0010 (13)	−0.0003 (11)
N3	0.055 (2)	0.0319 (16)	0.0214 (14)	0.0048 (14)	0.0045 (13)	−0.0049 (12)
N4	0.0420 (18)	0.0321 (16)	0.0287 (15)	0.0084 (13)	0.0021 (13)	−0.0035 (13)
N5	0.052 (2)	0.0353 (17)	0.0294 (16)	0.0109 (14)	0.0068 (14)	−0.0068 (13)
N6	0.0381 (18)	0.0389 (17)	0.0360 (17)	0.0006 (14)	−0.0005 (14)	−0.0041 (14)
O1	0.0584 (17)	0.0358 (14)	0.0310 (13)	0.0083 (12)	0.0053 (12)	−0.0092 (11)
O2	0.082 (2)	0.0459 (16)	0.0315 (15)	0.0122 (14)	0.0145 (14)	0.0010 (12)
O3	0.0611 (18)	0.0313 (13)	0.0317 (14)	0.0057 (12)	0.0040 (12)	−0.0034 (11)
O4	0.0538 (17)	0.0333 (13)	0.0307 (14)	0.0099 (11)	0.0010 (12)	−0.0005 (11)
O5	0.0567 (18)	0.0337 (14)	0.0334 (14)	−0.0041 (12)	−0.0006 (12)	−0.0066 (11)
O6	0.099 (3)	0.0498 (17)	0.0482 (18)	−0.0039 (17)	0.0139 (16)	−0.0173 (14)
C1	0.0318 (19)	0.0311 (18)	0.0282 (18)	−0.0018 (15)	−0.0008 (15)	−0.0066 (15)
C2	0.039 (2)	0.0291 (18)	0.0282 (18)	−0.0007 (15)	−0.0013 (15)	−0.0071 (14)

C3	0.062 (3)	0.033 (2)	0.034 (2)	0.0134 (18)	0.0006 (18)	−0.0034 (16)
C4	0.074 (3)	0.035 (2)	0.039 (2)	0.014 (2)	−0.002 (2)	0.0081 (17)
C5	0.064 (3)	0.041 (2)	0.0274 (19)	0.0053 (19)	0.0002 (18)	0.0015 (16)
C6	0.040 (2)	0.0290 (18)	0.0276 (18)	−0.0014 (15)	−0.0028 (15)	−0.0009 (14)
C7	0.046 (2)	0.0310 (19)	0.0296 (19)	0.0016 (16)	0.0031 (16)	−0.0030 (15)
C8	0.054 (2)	0.035 (2)	0.0306 (19)	−0.0005 (17)	−0.0002 (17)	−0.0015 (16)
C9	0.099 (4)	0.048 (2)	0.034 (2)	0.008 (2)	0.011 (2)	0.0040 (19)
C10	0.048 (2)	0.0324 (19)	0.031 (2)	0.0069 (16)	−0.0005 (17)	−0.0080 (16)
C11	0.067 (3)	0.044 (2)	0.043 (2)	0.020 (2)	−0.002 (2)	−0.0077 (18)
C12	0.050 (3)	0.060 (3)	0.052 (3)	−0.003 (2)	−0.012 (2)	0.008 (2)
C13	0.055 (3)	0.102 (4)	0.053 (3)	−0.014 (3)	−0.020 (2)	0.008 (3)
C14	0.060 (3)	0.101 (4)	0.062 (3)	−0.030 (3)	−0.006 (3)	−0.020 (3)
C15	0.061 (3)	0.065 (3)	0.086 (4)	−0.026 (2)	−0.011 (3)	−0.010 (3)
C16	0.044 (2)	0.051 (3)	0.055 (3)	−0.0125 (19)	−0.003 (2)	0.005 (2)
C17	0.067 (3)	0.058 (3)	0.058 (3)	−0.014 (2)	−0.005 (2)	−0.006 (2)
C18	0.109 (4)	0.053 (3)	0.057 (3)	−0.015 (3)	0.021 (3)	−0.007 (2)

Geometric parameters (Å, º)

Fe1—O5	1.922 (3)	C3—H3A	0.9300
Fe1—N4	2.107 (3)	C4—C5	1.381 (5)
Fe1—O4	2.142 (2)	C4—H4	0.9300
Fe1—N2	2.150 (3)	C5—C6	1.375 (5)
Fe1—O3	2.209 (2)	C5—H5A	0.9300
Fe1—N1	2.228 (3)	C6—C7	1.505 (4)
Fe1—N6	2.245 (3)	C8—C9	1.489 (5)
N1—C2	1.334 (4)	C9—H9A	0.9600
N1—C6	1.334 (4)	C9—H9B	0.9600
N2—C1	1.319 (4)	C9—H9C	0.9600
N2—N3	1.384 (4)	C10—C11	1.495 (5)
N3—C8	1.330 (4)	C11—H11A	0.9600
N3—H3	0.8600	C11—H11B	0.9600
N4—C7	1.325 (4)	C11—H11C	0.9600
N4—N5	1.391 (4)	C12—C13	1.377 (6)
N5—C10	1.320 (4)	C12—H12	0.9300
N5—H5	0.8600	C13—C14	1.361 (7)
N6—C16	1.327 (5)	C13—H13	0.9300
N6—C12	1.341 (4)	C14—C15	1.366 (6)
O1—C1	1.251 (4)	C14—H14	0.9300
O2—C7	1.238 (4)	C15—C16	1.374 (6)
O3—C8	1.252 (4)	C15—H15	0.9300
O4—C10	1.260 (4)	C16—H16	0.9300
O5—C17	1.363 (5)	C17—H17A	0.9600
O6—C18	1.424 (5)	C17—H17B	0.9600
O6—H6	0.8200	C17—H17C	0.9600
C1—C2	1.494 (4)	C18—H18A	0.9600
C2—C3	1.372 (5)	C18—H18B	0.9600
C3—C4	1.381 (5)	C18—H18C	0.9600

O5—Fe1—N4	93.67 (11)	C6—C5—C4	118.6 (3)
O5—Fe1—O4	94.66 (10)	C6—C5—H5A	120.7
N4—Fe1—O4	72.86 (9)	C4—C5—H5A	120.7
O5—Fe1—N2	96.21 (11)	N1—C6—C5	121.5 (3)
N4—Fe1—N2	138.16 (10)	N1—C6—C7	113.4 (3)
O4—Fe1—N2	145.91 (10)	C5—C6—C7	125.1 (3)
O5—Fe1—O3	88.85 (10)	O2—C7—N4	128.1 (3)
N4—Fe1—O3	149.43 (10)	O2—C7—C6	122.4 (3)
O4—Fe1—O3	76.57 (9)	N4—C7—C6	109.5 (3)
N2—Fe1—O3	71.46 (9)	O3—C8—N3	120.0 (3)
O5—Fe1—N1	93.58 (10)	O3—C8—C9	122.1 (3)
N4—Fe1—N1	69.58 (10)	N3—C8—C9	117.9 (3)
O4—Fe1—N1	141.95 (10)	C8—C9—H9A	109.5
N2—Fe1—N1	69.30 (10)	C8—C9—H9B	109.5
O3—Fe1—N1	140.72 (9)	H9A—C9—H9B	109.5
O5—Fe1—N6	172.22 (11)	C8—C9—H9C	109.5
N4—Fe1—N6	92.96 (11)	H9A—C9—H9C	109.5
O4—Fe1—N6	83.42 (10)	H9B—C9—H9C	109.5
N2—Fe1—N6	81.48 (11)	O4—C10—N5	119.8 (3)
O3—Fe1—N6	83.37 (10)	O4—C10—C11	121.7 (3)
N1—Fe1—N6	92.54 (10)	N5—C10—C11	118.6 (3)
C2—N1—C6	120.0 (3)	C10—C11—H11A	109.5
C2—N1—Fe1	120.3 (2)	C10—C11—H11B	109.5
C6—N1—Fe1	119.5 (2)	H11A—C11—H11B	109.5
C1—N2—N3	117.5 (3)	C10—C11—H11C	109.5
C1—N2—Fe1	125.9 (2)	H11A—C11—H11C	109.5
N3—N2—Fe1	116.18 (18)	H11B—C11—H11C	109.5
C8—N3—N2	114.9 (3)	N6—C12—C13	122.4 (4)
C8—N3—H3	122.5	N6—C12—H12	118.8
N2—N3—H3	122.5	C13—C12—H12	118.8
C7—N4—N5	116.8 (3)	C14—C13—C12	119.6 (4)
C7—N4—Fe1	126.6 (2)	C14—C13—H13	120.2
N5—N4—Fe1	115.8 (2)	C12—C13—H13	120.2
C10—N5—N4	114.3 (3)	C13—C14—C15	118.5 (4)
C10—N5—H5	122.9	C13—C14—H14	120.8
N4—N5—H5	122.9	C15—C14—H14	120.8
C16—N6—C12	117.2 (4)	C14—C15—C16	119.2 (5)
C16—N6—Fe1	122.0 (3)	C14—C15—H15	120.4
C12—N6—Fe1	120.1 (3)	C16—C15—H15	120.4
C8—O3—Fe1	116.7 (2)	N6—C16—C15	123.2 (4)
C10—O4—Fe1	117.0 (2)	N6—C16—H16	118.4
C17—O5—Fe1	125.7 (2)	C15—C16—H16	118.4
C18—O6—H6	109.5	O5—C17—H17A	109.5
O1—C1—N2	128.4 (3)	O5—C17—H17B	109.5
O1—C1—C2	121.3 (3)	H17A—C17—H17B	109.5
N2—C1—C2	110.3 (3)	O5—C17—H17C	109.5
N1—C2—C3	121.6 (3)	H17A—C17—H17C	109.5

N1—C2—C1	113.5 (3)	H17B—C17—H17C	109.5
C3—C2—C1	125.0 (3)	O6—C18—H18A	109.5
C2—C3—C4	118.8 (3)	O6—C18—H18B	109.5
C2—C3—H3A	120.6	H18A—C18—H18B	109.5
C4—C3—H3A	120.6	O6—C18—H18C	109.5
C3—C4—C5	119.5 (3)	H18A—C18—H18C	109.5
C3—C4—H4	120.3	H18B—C18—H18C	109.5
C5—C4—H4	120.3		

O5—Fe1—N1—C2	91.5 (3)	N4—Fe1—O4—C10	−5.2 (3)
N4—Fe1—N1—C2	−175.9 (3)	N2—Fe1—O4—C10	−164.4 (3)
O4—Fe1—N1—C2	−166.3 (2)	O3—Fe1—O4—C10	175.0 (3)
N2—Fe1—N1—C2	−3.8 (2)	N1—Fe1—O4—C10	−14.6 (4)
O3—Fe1—N1—C2	−1.1 (3)	N6—Fe1—O4—C10	−100.3 (3)
N6—Fe1—N1—C2	−83.7 (3)	N4—Fe1—O5—C17	−159.1 (3)
O5—Fe1—N1—C6	−82.8 (3)	O4—Fe1—O5—C17	127.8 (3)
N4—Fe1—N1—C6	9.8 (2)	N2—Fe1—O5—C17	−19.8 (3)
O4—Fe1—N1—C6	19.5 (3)	O3—Fe1—O5—C17	51.4 (3)
N2—Fe1—N1—C6	−178.1 (3)	N1—Fe1—O5—C17	−89.3 (3)
O3—Fe1—N1—C6	−175.3 (2)	N3—N2—C1—O1	0.5 (6)
N6—Fe1—N1—C6	102.0 (3)	Fe1—N2—C1—O1	−171.7 (3)
O5—Fe1—N2—C1	−93.7 (3)	N3—N2—C1—C2	179.0 (3)
N4—Fe1—N2—C1	8.9 (4)	Fe1—N2—C1—C2	6.8 (4)
O4—Fe1—N2—C1	158.5 (2)	C6—N1—C2—C3	2.2 (5)
O3—Fe1—N2—C1	179.6 (3)	Fe1—N1—C2—C3	−172.0 (3)
N1—Fe1—N2—C1	−2.2 (3)	C6—N1—C2—C1	−177.5 (3)
N6—Fe1—N2—C1	93.8 (3)	Fe1—N1—C2—C1	8.3 (4)
O5—Fe1—N2—N3	94.0 (2)	O1—C1—C2—N1	169.5 (3)
N4—Fe1—N2—N3	−163.4 (2)	N2—C1—C2—N1	−9.2 (4)
O4—Fe1—N2—N3	−13.9 (4)	O1—C1—C2—C3	−10.3 (6)
O3—Fe1—N2—N3	7.3 (2)	N2—C1—C2—C3	171.1 (4)
N1—Fe1—N2—N3	−174.5 (3)	N1—C2—C3—C4	−0.7 (6)
N6—Fe1—N2—N3	−78.5 (2)	C1—C2—C3—C4	179.0 (4)
C1—N2—N3—C8	179.5 (3)	C2—C3—C4—C5	−1.0 (6)
Fe1—N2—N3—C8	−7.5 (4)	C3—C4—C5—C6	1.1 (7)
O5—Fe1—N4—C7	81.0 (3)	C2—N1—C6—C5	−2.1 (5)
O4—Fe1—N4—C7	174.7 (3)	Fe1—N1—C6—C5	172.1 (3)
N2—Fe1—N4—C7	−22.6 (4)	C2—N1—C6—C7	177.7 (3)
O3—Fe1—N4—C7	174.9 (3)	Fe1—N1—C6—C7	−8.0 (4)
N1—Fe1—N4—C7	−11.5 (3)	C4—C5—C6—N1	0.4 (6)
N6—Fe1—N4—C7	−103.1 (3)	C4—C5—C6—C7	−179.4 (4)
O5—Fe1—N4—N5	−88.6 (2)	N5—N4—C7—O2	−0.2 (6)
O4—Fe1—N4—N5	5.1 (2)	Fe1—N4—C7—O2	−169.8 (3)
N2—Fe1—N4—N5	167.8 (2)	N5—N4—C7—C6	−179.7 (3)
O3—Fe1—N4—N5	5.3 (4)	Fe1—N4—C7—C6	10.7 (4)
N1—Fe1—N4—N5	178.9 (3)	N1—C6—C7—O2	179.6 (4)
N6—Fe1—N4—N5	87.3 (2)	C5—C6—C7—O2	−0.5 (6)
C7—N4—N5—C10	−175.5 (3)	N1—C6—C7—N4	−0.8 (4)

Fe1—N4—N5—C10	−4.8 (4)	C5—C6—C7—N4	179.0 (4)
N4—Fe1—N6—C16	65.6 (3)	Fe1—O3—C8—N3	5.4 (5)
O4—Fe1—N6—C16	138.0 (3)	Fe1—O3—C8—C9	−174.0 (3)
N2—Fe1—N6—C16	−72.7 (3)	N2—N3—C8—O3	1.3 (5)
O3—Fe1—N6—C16	−144.8 (3)	N2—N3—C8—C9	−179.3 (3)
N1—Fe1—N6—C16	−4.0 (3)	Fe1—O4—C10—N5	4.4 (5)
N4—Fe1—N6—C12	−124.6 (3)	Fe1—O4—C10—C11	−175.9 (3)
O4—Fe1—N6—C12	−52.3 (3)	N4—N5—C10—O4	0.2 (5)
N2—Fe1—N6—C12	97.1 (3)	N4—N5—C10—C11	−179.4 (3)
O3—Fe1—N6—C12	24.9 (3)	C16—N6—C12—C13	2.2 (6)
N1—Fe1—N6—C12	165.7 (3)	Fe1—N6—C12—C13	−168.0 (3)
O5—Fe1—O3—C8	−103.8 (3)	N6—C12—C13—C14	−0.5 (7)
N4—Fe1—O3—C8	161.0 (3)	C12—C13—C14—C15	−1.5 (7)
O4—Fe1—O3—C8	161.2 (3)	C13—C14—C15—C16	1.8 (7)
N2—Fe1—O3—C8	−6.8 (3)	C12—N6—C16—C15	−1.9 (6)
N1—Fe1—O3—C8	−9.5 (4)	Fe1—N6—C16—C15	168.1 (3)
N6—Fe1—O3—C8	76.4 (3)	C14—C15—C16—N6	−0.1 (7)
O5—Fe1—O4—C10	87.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{i}	0.86	1.94	2.780 (3)	167
N5—H5···O6^{ii}	0.86	1.98	2.830 (4)	167
O6—H6···O5^{iii}	0.82	1.90	2.718 (3)	172

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