

catena-Poly[[[diaquairon(II)]- μ -pyridine-2,5-dicarboxylato-[tetraaquairon(II)]- μ -pyridine-2,5-dicarboxylato] tetrahydrate]

Hai-Yun Xu,* Huai-Ling Ma, Mao-Tian Xu, Wen-Xian Zhao and Bao-Guo Guo

Department of Chemistry, Shangqiu Normal College, 476000 Shangqiu, Henan, People's Republic of China

Correspondence e-mail: xuhyun@yahoo.cn

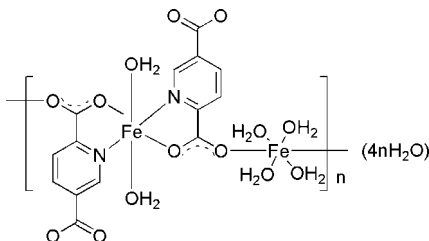
Received 22 December 2007; accepted 20 January 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.043; wR factor = 0.125; data-to-parameter ratio = 12.0.

In the crystal structure of the title compound, $\{[\text{Fe}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{H}_2\text{O})_6] \cdot 4\text{H}_2\text{O}\}_n$, there are two types of coordination for the Fe^{II} atoms. One Fe^{II} atom is in a distorted octahedral N_2O_4 environment, with two chelating rings from the pyridine-dicarboxylate ligands and two O atoms from the water molecules, while the other is in a distorted octahedral O_6 environment with two O atoms from the pyridinedicarboxylate ligands and four O atoms from the water molecules. Both Fe^{II} atoms lie on crystallographic centers of symmetry. The complex possesses an infinite chain structure running along the [101] direction. These chains are interconnected by the uncoordinated water molecules through $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related literature, see: Hill (1998); Liang *et al.* (2001); Mitzi *et al.* (1995); Moler *et al.* (2001); Zeng *et al.* (2003); Xu *et al.* (2004).



Experimental

Crystal data

$[\text{Fe}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{H}_2\text{O})_6] \cdot 4\text{H}_2\text{O}$
 $M_r = 622.06$
 Triclinic, $P\bar{1}$
 $a = 7.098$ (3) Å
 $b = 8.922$ (3) Å
 $c = 9.720$ (2) Å

$\alpha = 90.942$ (6)°
 $\beta = 101.375$ (6)°
 $\gamma = 108.112$ (5)°
 $V = 571.6$ (3) Å³
 $Z = 1$

Mo $K\alpha$ radiation
 $\mu = 1.36$ mm⁻¹
 $T = 298$ (2) K
 $0.21 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.763$, $T_{\text{max}} = 0.792$

2866 measured reflections
 1989 independent reflections
 1757 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.062$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.124$
 $S = 1.06$
 1989 reflections

166 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O9}-\text{H9B}\cdots\text{O8}$	0.85	2.32	3.159 (6)	171
$\text{O9}-\text{H9A}\cdots\text{O6}^{\text{i}}$	0.85	2.06	2.849 (5)	154
$\text{O8}-\text{H8B}\cdots\text{O5}^{\text{ii}}$	0.85	2.55	3.204 (4)	134
$\text{O8}-\text{H8B}\cdots\text{O4}^{\text{iii}}$	0.85	2.51	3.171 (4)	136
$\text{O8}-\text{H8A}\cdots\text{O3}$	0.85	2.55	3.177 (4)	132
$\text{O8}-\text{H8A}\cdots\text{O2}$	0.85	2.44	3.201 (4)	149
$\text{O5}-\text{H5B}\cdots\text{O7}^{\text{i}}$	0.85	2.22	2.706 (3)	116
$\text{O2}-\text{H2B}\cdots\text{O9}^{\text{iii}}$	0.85	1.94	2.657 (5)	141
$\text{O2}-\text{H2A}\cdots\text{O4}^{\text{iv}}$	0.85	1.99	2.758 (3)	150
$\text{O1}-\text{H1B}\cdots\text{O6}^{\text{v}}$	0.85	1.92	2.715 (3)	156
$\text{O1}-\text{H1A}\cdots\text{O8}^{\text{ii}}$	0.85	2.06	2.822 (4)	148

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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.

The authors thank the Natural Science Foundation of Henan Province (No. 0511020300) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2270).

References

- Hill, C. L. (1998). *Chem. Rev.* **98**, 1–390.
 Liang, Y.-C., Hong, M.-C., Su, W.-P., Cao, R. & Zhang, W.-J. (2001). *Inorg. Chem.* **40**, 4574–4582.
 Mitzi, D. B., Wang, S., Field, C. A., Chess, C. A. & Guloy, A. M. (1995). *Science*, **267**, 1473–1476.
 Moler, D. B., Li, H., Chen, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Xu, Y., Han, L., Lin, Z.-Z., Liu, C.-P., Yuan, D.-Q., Zhou, Y.-F. & Hong, M.-C. (2004). *Eur. J. Inorg. Chem.* pp. 4457–4462.
 Zeng, M.-H., Gao, S., Yu, X.-L. & Chen, X.-M. (2003). *New J. Chem.* **27**, 1599–1602.

supporting information

Acta Cryst. (2008). E64, m413 [doi:10.1107/S1600536808002043]

catena-Poly[[[diaquairon(II)]- μ -pyridine-2,5-dicarboxylato-[tetraaquairon(II)]- μ -pyridine-2,5-dicarboxylato] tetrahydrate]

Hai-Yun Xu, Huai-Ling Ma, Mao-Tian Xu, Wen-Xian Zhao and Bao-Guo Guo

S1. Comment

Extended frameworks of coordination polymers based on transition metal ions and multifunctional bridging ligands are currently of great interest because of their intriguing topologies and their potential applications (Hill, 1998; Moler *et al.*, 2001; Mitzi *et al.*, 1995). Multi-carboxylate ligands may exhibit various coordination modes to furnish various structures. Recently, many transition metal-organic polymers constructed with multi-carboxylate ligands show various novel topology and potential applications in catalysis, materials chemistry and biochemistry (Zeng *et al.*, 2003; Xu *et al.*, 2004; Liang *et al.*, 2001). Pyridine-2,5-dicarboxylic acid (H_2pydc) has unique features because of the presence of two carboxylate groups (O donor atoms) and the pyridine ring (N donor atom), which aids to increase the dimensionality of the assembled covalent network. Therefore, it is most likely that $pydc$ will form low symmetric structures with metals. In this paper, we report the preparation and crystal structure of a new three-dimensional supramolecular complex $[Fe_2(pydc)_2(H_2O)_2] \cdot 4H_2O$, (I).

In the complex, (I), there exist two types of coordination geometries around the Fe(II) ions. The Fe1 ions are hexacoordinated in a N_2O_4 environment with two chelating rings from the $pydc$ ligands and two oxygen atoms from the water molecules. The Fe2 ions are also hexacoordinated in an O_6 environment with two oxygen atoms from the $pydc$ ligands and four oxygen atoms from the water molecules. All Fe atoms lie on a crystallographic center of symmetry and the ligand lies on a crystallographic twofold axis. A perspective view of the local coordination environments around the Fe(II) atoms of (I) is shown in Fig. 1. For Fe1 and Fe2, the bond distances of Fe—O (water oxygen), 2.071–2.100 Å, are similar with those of Fe—O (carboxylate oxygen), 2.058–2.080 Å. As presented in Fig. 2, the two kinds of geometries around Fe(II) ions are arranged alternatively to give the one-dimensional polymeric chain. Interestingly, all Fe atoms of one polymeric chain are situated on one line and the neighboring Fe(II) atoms are *syn-anti* carboxylato bridged with the distance of 5.423 Å. These chains are interconnected by the uncoordinated water molecules through O—H \cdots O hydrogen-bonding interactions and form a two-dimensional layer structure. A three-dimensional supramolecular network is obtained through O—H \cdots O hydrogen-bonding interactions in the layers.

S2. Experimental

A mixture of H_2pydc (0.34 g, 2 mmol), KOH (0.23 g, 4 mmol) and $FeSO_4 \cdot 7H_2O$ (0.55 g, 2 mmol) in 15 ml of MeOH/ H_2O (v/v, 1:1) was sealed in a 25-ml stainless-steel reactor with a teflon liner and was heated at 453 K for 72 h under autogenous pressure. Slow cooling to room temperature yielded 0.36 g (yield 40%) of block red crystals. Anal. Calc. for $C_7H_{13}NO_9Fe$ (%): C 27.03, H 4.21, N 4.50. Found (%): C 27.14, H 4.46, N 4.36.

S3. Refinement

The H atoms were included in the riding-model approximation with C—H = 0.93 Å and O—H = 0.85 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$. Hydroxyl H atoms were allowed to rotate to best fit the experimental electron density.

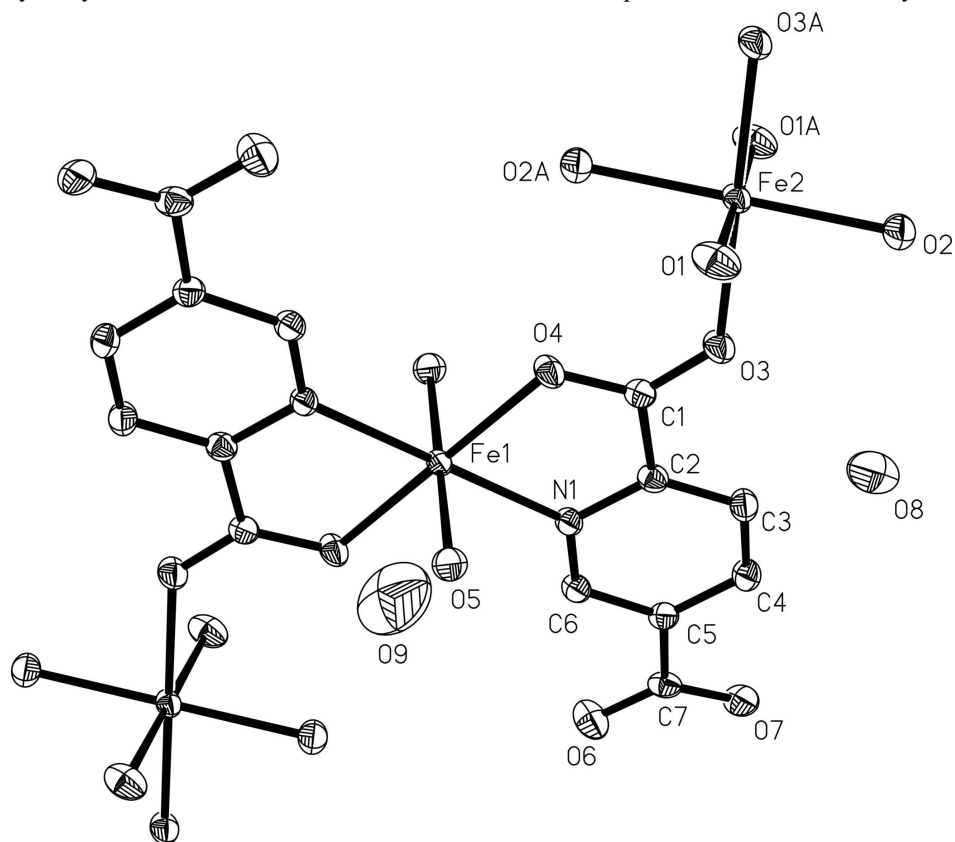


Figure 1

Part of the polymeric structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity. The suffix A corresponds to symmetry code (2 - x, 1 - y, 1 - z).

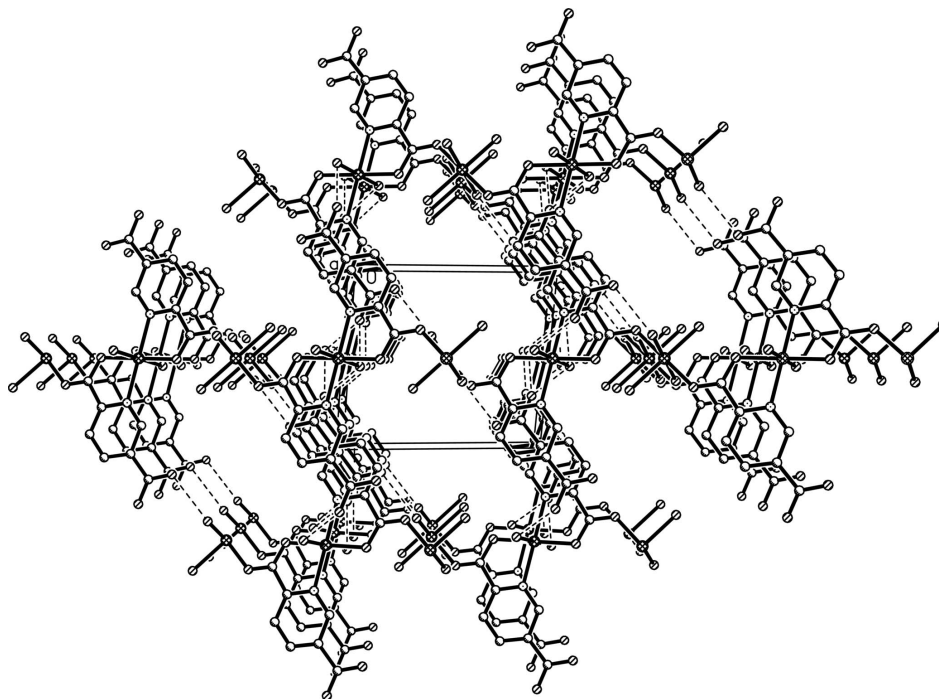


Figure 2

The three-dimensional supramolecular structure of the title compound. Hydrogen bonds are shown by dashed lines.

catena-Poly[[[diaquairon(II)]- μ -pyridine-2,5-dicarboxylato- [tetraquairon(II)]- μ -pyridine-2,5-dicarboxylato] tetrahydrate]

Crystal data

$[\text{Fe}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{H}_2\text{O})_6] \cdot 4\text{H}_2\text{O}$

$M_r = 622.06$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.098$ (3) Å

$b = 8.922$ (3) Å

$c = 9.720$ (2) Å

$\alpha = 90.942$ (6)°

$\beta = 101.375$ (6)°

$\gamma = 108.112$ (5)°

$V = 571.6$ (3) Å³

$Z = 1$

$F(000) = 320$

$D_x = 1.807$ Mg m⁻³

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

Cell parameters from 714 reflections

$\theta = 2.4$ – 28.2 °

$\mu = 1.36$ mm⁻¹

$T = 298$ K

Block, red

$0.21 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.763$, $T_{\max} = 0.792$

2866 measured reflections

1989 independent reflections

1757 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.1$ °

$h = -8 \rightarrow 6$

$k = -10 \rightarrow 10$

$l = -11 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.124$
 $S = 1.06$
 1989 reflections
 166 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
 $w = 1/[\sigma^2(F_o^2) + (0.081P)^2 + 0.2244P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.5000	0.5000	0.0000	0.0222 (2)
Fe2	1.0000	0.5000	0.5000	0.0258 (2)
C1	0.6446 (4)	0.3738 (3)	0.2523 (3)	0.0270 (6)
C2	0.4924 (4)	0.2309 (3)	0.1667 (3)	0.0275 (6)
C3	0.4514 (5)	0.0824 (3)	0.2147 (3)	0.0330 (7)
H3	0.5126	0.0679	0.3050	0.040*
C4	0.3189 (5)	-0.0438 (3)	0.1270 (3)	0.0331 (7)
H4	0.2889	-0.1449	0.1579	0.040*
C5	0.2302 (4)	-0.0216 (3)	-0.0065 (3)	0.0278 (6)
C6	0.2767 (4)	0.1328 (3)	-0.0474 (3)	0.0279 (6)
H6	0.2161	0.1496	-0.1372	0.033*
C7	0.0905 (4)	-0.1587 (4)	-0.1093 (3)	0.0318 (7)
N1	0.4039 (3)	0.2565 (3)	0.0369 (3)	0.0261 (5)
O1	0.8315 (4)	0.6187 (3)	0.5803 (3)	0.0448 (6)
H1A	0.7132	0.6145	0.5373	0.054*
H1B	0.9150	0.7017	0.6279	0.054*
O2	0.9411 (3)	0.3350 (3)	0.6494 (2)	0.0425 (6)
H2B	0.8576	0.2419	0.6286	0.051*
H2A	1.0460	0.3570	0.7156	0.051*
O3	0.7348 (3)	0.3533 (2)	0.3701 (2)	0.0352 (5)
O4	0.6748 (3)	0.5047 (2)	0.1970 (2)	0.0334 (5)
O5	0.2787 (3)	0.5429 (3)	0.0954 (2)	0.0361 (5)
H5A	0.1792	0.5354	0.0276	0.043*
H5B	0.2288	0.4806	0.1537	0.043*
O6	0.0097 (4)	-0.1287 (3)	-0.2262 (3)	0.0473 (6)

O7	0.0653 (4)	-0.2939 (3)	-0.0688 (3)	0.0430 (6)
O8	0.4663 (4)	0.2880 (4)	0.6019 (3)	0.0640 (8)
H8B	0.4601	0.3105	0.6859	0.077*
H8A	0.5871	0.3270	0.5904	0.077*
O9	0.1591 (7)	-0.0327 (5)	0.4428 (6)	0.1112 (15)
H9B	0.2489	0.0471	0.4912	0.133*
H9A	0.1463	0.0205	0.3718	0.133*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0226 (3)	0.0153 (3)	0.0243 (3)	0.0050 (2)	-0.0034 (2)	-0.0004 (2)
Fe2	0.0269 (4)	0.0200 (3)	0.0247 (3)	0.0056 (2)	-0.0043 (2)	-0.0003 (2)
C1	0.0253 (14)	0.0248 (14)	0.0301 (15)	0.0088 (12)	0.0027 (11)	-0.0011 (11)
C2	0.0261 (14)	0.0260 (14)	0.0284 (15)	0.0082 (12)	0.0021 (11)	-0.0013 (11)
C3	0.0369 (17)	0.0282 (15)	0.0302 (16)	0.0083 (13)	0.0019 (13)	0.0059 (12)
C4	0.0357 (16)	0.0215 (14)	0.0403 (17)	0.0090 (13)	0.0041 (13)	0.0059 (12)
C5	0.0251 (14)	0.0225 (14)	0.0355 (16)	0.0079 (12)	0.0054 (12)	0.0003 (12)
C6	0.0277 (15)	0.0226 (13)	0.0314 (15)	0.0088 (12)	0.0006 (12)	-0.0004 (11)
C7	0.0242 (14)	0.0258 (15)	0.0432 (18)	0.0083 (12)	0.0023 (13)	-0.0049 (13)
N1	0.0259 (12)	0.0187 (11)	0.0308 (13)	0.0071 (10)	-0.0003 (10)	0.0014 (9)
O1	0.0403 (13)	0.0383 (13)	0.0492 (14)	0.0153 (11)	-0.0089 (11)	-0.0151 (11)
O2	0.0407 (13)	0.0349 (12)	0.0411 (13)	0.0033 (10)	-0.0026 (10)	0.0113 (10)
O3	0.0366 (12)	0.0278 (11)	0.0308 (11)	0.0047 (9)	-0.0072 (9)	0.0010 (8)
O4	0.0367 (12)	0.0228 (10)	0.0314 (11)	0.0071 (9)	-0.0096 (9)	-0.0011 (8)
O5	0.0320 (11)	0.0320 (12)	0.0439 (13)	0.0104 (10)	0.0072 (10)	0.0046 (10)
O6	0.0572 (15)	0.0302 (12)	0.0434 (14)	0.0136 (11)	-0.0134 (11)	-0.0088 (10)
O7	0.0367 (13)	0.0198 (11)	0.0632 (16)	0.0040 (10)	-0.0020 (11)	-0.0008 (10)
O8	0.0469 (16)	0.075 (2)	0.066 (2)	0.0196 (16)	0.0038 (14)	0.0019 (16)
O9	0.116 (3)	0.054 (2)	0.163 (5)	0.019 (2)	0.041 (3)	0.000 (2)

Geometric parameters (Å, °)

Fe1—O4	2.058 (2)	C4—C5	1.372 (4)
Fe1—O4 ⁱ	2.058 (2)	C4—H4	0.9300
Fe1—O5 ⁱ	2.100 (2)	C5—C6	1.397 (4)
Fe1—O5	2.100 (2)	C5—C7	1.515 (4)
Fe1—N1	2.125 (2)	C6—N1	1.328 (4)
Fe1—N1 ⁱ	2.125 (2)	C6—H6	0.9300
Fe2—O1	2.071 (2)	C7—O6	1.241 (4)
Fe2—O1 ⁱⁱ	2.071 (2)	C7—O7	1.245 (4)
Fe2—O3 ⁱⁱ	2.080 (2)	O1—H1A	0.8499
Fe2—O3	2.080 (2)	O1—H1B	0.8499
Fe2—O2	2.092 (2)	O2—H2B	0.8500
Fe2—O2 ⁱⁱ	2.092 (2)	O2—H2A	0.8501
C1—O3	1.242 (3)	O5—H5A	0.8499
C1—O4	1.268 (4)	O5—H5B	0.8500
C1—C2	1.496 (4)	O8—H8B	0.8500

C2—N1	1.351 (4)	O8—H8A	0.8499
C2—C3	1.376 (4)	O9—H9B	0.8499
C3—C4	1.368 (4)	O9—H9A	0.8500
C3—H3	0.9300		
O4—Fe1—O4 ⁱ	180.00 (11)	N1—C2—C1	115.5 (2)
O4—Fe1—O5 ⁱ	90.89 (9)	C3—C2—C1	122.3 (3)
O4 ⁱ —Fe1—O5 ⁱ	89.11 (9)	C4—C3—C2	118.8 (3)
O4—Fe1—O5	89.11 (9)	C4—C3—H3	120.6
O4 ⁱ —Fe1—O5	90.89 (9)	C2—C3—H3	120.6
O5 ⁱ —Fe1—O5	180.00 (6)	C3—C4—C5	120.2 (3)
O4—Fe1—N1	79.00 (8)	C3—C4—H4	119.9
O4 ⁱ —Fe1—N1	101.00 (8)	C5—C4—H4	119.9
O5 ⁱ —Fe1—N1	88.20 (9)	C4—C5—C6	117.9 (3)
O5—Fe1—N1	91.80 (9)	C4—C5—C7	121.9 (3)
O4—Fe1—N1 ⁱ	101.00 (8)	C6—C5—C7	120.2 (3)
O4 ⁱ —Fe1—N1 ⁱ	79.00 (8)	N1—C6—C5	122.5 (3)
O5 ⁱ —Fe1—N1 ⁱ	91.80 (9)	N1—C6—H6	118.7
O5—Fe1—N1 ⁱ	88.20 (9)	C5—C6—H6	118.7
N1—Fe1—N1 ⁱ	180.0	O6—C7—O7	125.1 (3)
O1—Fe2—O1 ⁱⁱ	180.00 (12)	O6—C7—C5	118.1 (3)
O1—Fe2—O3 ⁱⁱ	90.59 (9)	O7—C7—C5	116.8 (3)
O1 ⁱⁱ —Fe2—O3 ⁱⁱ	89.41 (9)	C6—N1—C2	118.4 (2)
O1—Fe2—O3	89.41 (9)	C6—N1—Fe1	129.8 (2)
O1 ⁱⁱ —Fe2—O3	90.59 (9)	C2—N1—Fe1	111.81 (18)
O3 ⁱⁱ —Fe2—O3	180.0	Fe2—O1—H1A	122.3
O1—Fe2—O2	89.15 (10)	Fe2—O1—H1B	107.1
O1 ⁱⁱ —Fe2—O2	90.85 (10)	H1A—O1—H1B	122.4
O3 ⁱⁱ —Fe2—O2	93.74 (9)	Fe2—O2—H2B	122.9
O3—Fe2—O2	86.26 (9)	Fe2—O2—H2A	108.0
O1—Fe2—O2 ⁱⁱ	90.85 (10)	H2B—O2—H2A	122.9
O1 ⁱⁱ —Fe2—O2 ⁱⁱ	89.15 (10)	C1—O3—Fe2	129.74 (18)
O3 ⁱⁱ —Fe2—O2 ⁱⁱ	86.26 (9)	C1—O4—Fe1	116.24 (18)
O3—Fe2—O2 ⁱⁱ	93.74 (9)	Fe1—O5—H5A	104.8
O2—Fe2—O2 ⁱⁱ	180.0	Fe1—O5—H5B	119.7
O3—C1—O4	125.5 (3)	H5A—O5—H5B	105.0
O3—C1—C2	117.1 (2)	H8B—O8—H8A	110.3
O4—C1—C2	117.3 (2)	H9B—O9—H9A	91.5
N1—C2—C3	122.2 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O9—H9B \cdots O8	0.85	2.32	3.159 (6)	171
O9—H9A \cdots O6 ⁱⁱⁱ	0.85	2.06	2.849 (5)	154
O8—H8B \cdots O5 ^{iv}	0.85	2.55	3.204 (4)	134

O8—H8B···O4 ^{iv}	0.85	2.51	3.171 (4)	136
O8—H8A···O3	0.85	2.55	3.177 (4)	132
O8—H8A···O2	0.85	2.44	3.201 (4)	149
O5—H5B···O7 ⁱⁱⁱ	0.85	2.22	2.706 (3)	116
O2—H2B···O9 ^v	0.85	1.94	2.657 (5)	141
O2—H2A···O4 ⁱⁱ	0.85	1.99	2.758 (3)	150
O1—H1B···O6 ^{vi}	0.85	1.92	2.715 (3)	156
O1—H1A···O8 ^{iv}	0.85	2.06	2.822 (4)	148

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