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Poly[[(μ_4-5-aminoisophthalato)aqua-iron(II)] dihydrate]

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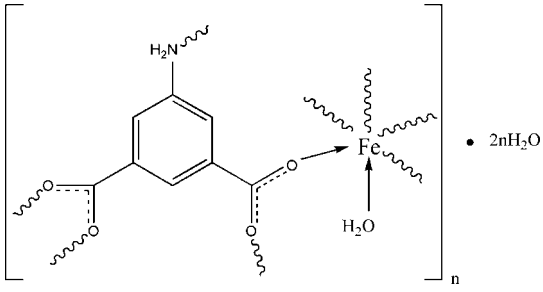
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.090; data-to-parameter ratio = 11.7.

In the title three-dimensional coordination polymer, $\{[Fe(C_8H_5NO_4)(H_2O)]\cdot 2H_2O\}_n$, the Fe^{II} atom exhibits a distorted octahedral geometry, being coordinated by one N and four O atoms from four 5-aminoisophthalate ligands and one water molecule. In addition, the crystal structure is stabilized by numerous O—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Wu *et al.* (2002); Zeng *et al.* (2007); Liao *et al.* (2006); Li *et al.* (2006).



Experimental

Crystal data

$[Fe(C_8H_5NO_4)(H_2O)]\cdot 2H_2O$
M_r = 289.03
Triclinic, $P\overline{1}$
a = 7.7418 (2) Å
b = 8.5972 (2) Å
c = 8.6938 (2) Å
α = 85.560 (1)°
β = 76.058 (1)°
γ = 66.610 (1)°
V = 515.34 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.17 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.755, T_{max} = 0.786
5025 measured reflections
2009 independent reflections
1895 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.090
S = 1.05
2009 reflections
172 parameters
11 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—O1	2.1040 (16)	Fe1—O4^{ii}	2.2387 (17)
Fe1—O2^{i}	2.1364 (16)	Fe1—O3^{ii}	2.3416 (16)
Fe1—O1W	2.1458 (17)	Fe1—N1^{iii}	2.376 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H3W···O2W^{iv}	0.844 (10)	2.377 (9)	2.892 (5)	119.9 (9)
O3W—H5W···O2^{v}	0.843 (10)	2.09 (2)	2.852 (3)	151 (4)
O3W—H6W···O2W^{vi}	0.840 (10)	2.071 (19)	2.865 (3)	157 (3)
O2W—H4W···O4^{vii}	0.842 (10)	2.05 (2)	2.816 (3)	151 (3)
O1W—H2W···O2W^{viii}	0.809 (9)	1.943 (12)	2.745 (3)	171 (3)
O1W—H1W···O3^{ix}	0.815 (10)	1.914 (14)	2.705 (3)	163 (4)
N1—H1B···O3W	0.90	2.19	3.015 (3)	153

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: *SHELXL97*.

The authors thank Guang Dong Ocean University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2125).

References

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, X.-J., Yuan, D.-Q., Zhang, X.-D. & Cao, R. (2006). *J. Coord. Chem.* **59**, 969–976.
Liao, Q.-X. & Yao, Y.-G. (2006). *Chin. J. Struct. Chem.* **25**, 465–468.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wu, C.-D., Lu, C.-Z., Yang, W.-B., Zhuang, H.-H. & Huang, J.-S. (2002). *Inorg. Chem.* **41**, 3302–3307.
Zeng, R.-H., Fang, Z.-Q., Sun, F., Jiang, L.-S. & Tang, Y.-W. (2007). *Acta Cryst.* E**63**, m1813–m1814.

supporting information

Acta Cryst. (2008). E**64**, m549 [doi:10.1107/S1600536808006326]

Poly[[(μ_4-5-aminoisophthalato)aquairon(II)] dihydrate]

Wen-Dong Song, Jian-Bin Yan, Li-Li Ji and Hao Wang

S1. Comment

5-Aminoisophthalatic acid is a good example of a bridging ligand that can link metal centres into extended networks, and a number of one-, two- and three- dimensional coordination frameworks have been generated (Zeng *et al.*, 2007; Wu *et al.*, 2002; Liao *et al.* 2006). Recently, we have obtained the title three-dimensional iron polymer, (I), and its crystal structure is reported here. This complex is isostructural with the Mn^{II} complex reported by Liao and Yao (2006) and by Li *et al.* (2006).

In the structure of (I) each Fe^{II} atom is coordinated by four O atoms from three 5-aminoisophthalate ligands, one N atom from another 5-aminoisophthalate ligand and one water molecule, and displays a distorted octahedral coordination geometry. The 5-aminoisophthalate ligands bridge iron ions to form a three-dimensional network (Fig. 2). Moreover, there are O—H···O and N—H···O hydrogen-bonding interactions within the three-dimensional structure connecting the carboxyl O atoms and amino N atoms of 5-aminoisophthalate ligands, the coordinating water molecules and water of crystallization (Table 2).

S2. Experimental

A mixture of $FeCl_2$ (0.5 mmol), 5-aminoisophthalatic acid (0.5 mmol), NaOH (1 mmol) and H_2O (12 ml) was placed in a 23 ml Teflon reactor, which was heated at 433 K for three days and then cooled to room temperature at a rate of 5 K h^{-1}. Single crystals were obtained after washing with water and drying in air.

S3. Refinement

All H atoms attached to C and N atoms were fixed geometrically and treated as riding on their parent atoms with C—H = 0.93 Å (aromatic), N—H = 0.90 Å and U_{iso}(H) = 1.2 U_{eq}(C,*N*). H atoms from water molecules were located in difference Fourier maps and included in the subsequent refinement using restraints [O—H= 0.82 (1) Å and H···H= 1.34 (2) Å] with U_{iso}(H) = 1.5U_{eq}(O).

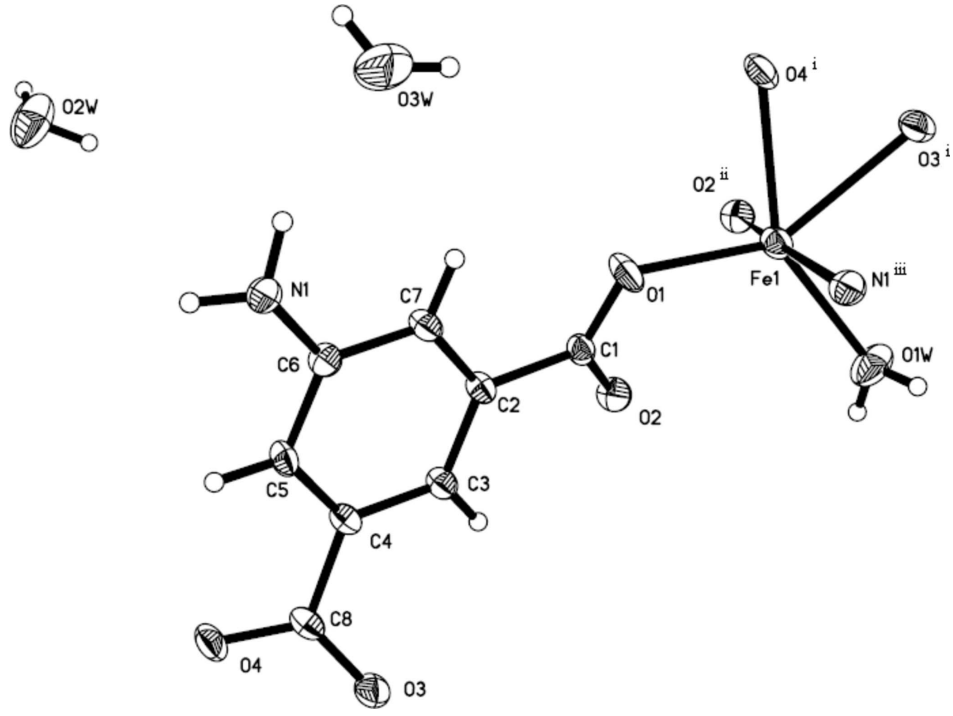


Figure 1

The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) -1 + *x*, *y*, *z* + 1; (ii) -*x*, 2 - *y*, 2 - *z*; (iii) 1 - *x*, 1 - *y*, 2 - *z*]]

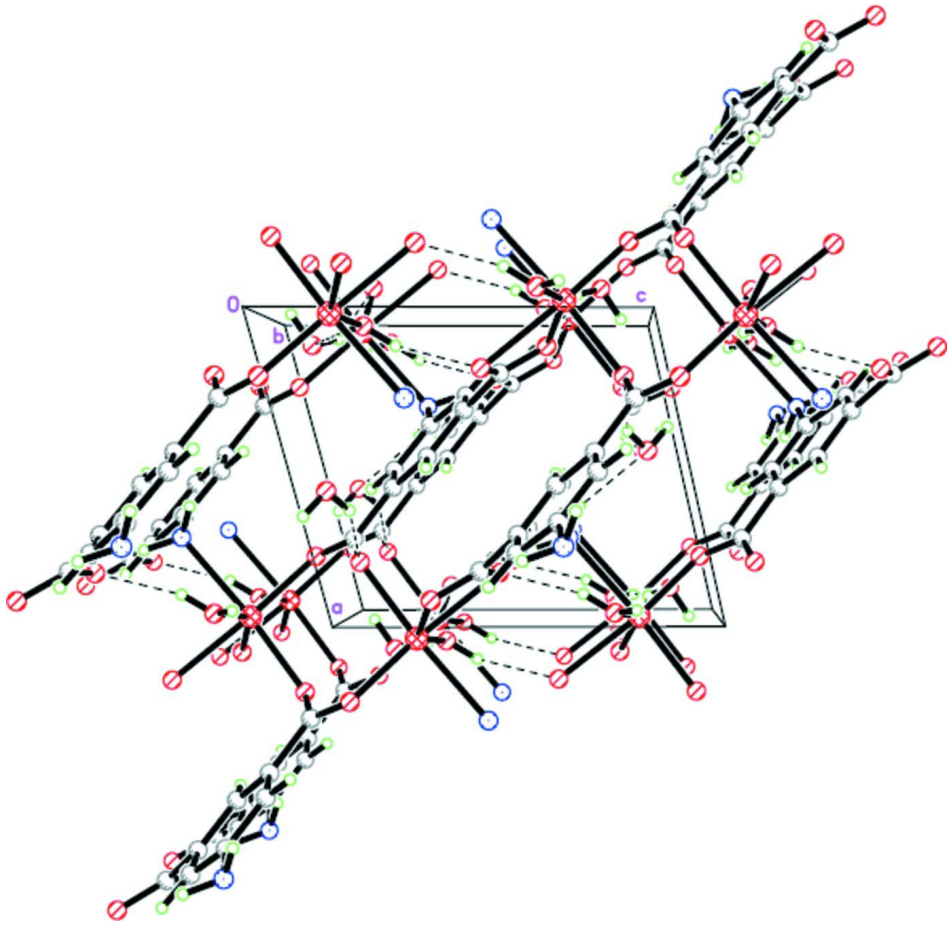


Figure 2

The three-dimensional network structure of the title compound, viewed along the *b* axis.

Poly[[(μ_4-5-Aminoisophthalato)aquairon(II)] dihydrate]

Crystal data

$[Fe(C_8H_5NO_4)(H_2O)]\cdot 2H_2O$
$M_r = 289.03$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.7418$ (2) Å
$b = 8.5972$ (2) Å
$c = 8.6938$ (2) Å
$\alpha = 85.560$ (1)°
$\beta = 76.058$ (1)°
$\gamma = 66.610$ (1)°
$V = 515.34$ (2) Å^3
$Z = 2$
$F(000) = 296$
$D_x = 1.863$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1800 reflections
$\theta = 1.4$–28.0°
$\mu = 1.49$ mm^{-1}
$T = 293$ K
Block, red
0.20 × 0.18 × 0.17 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.755$, $T_{max} = 0.786$
5025 measured reflections
2009 independent reflections

1895 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$

$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.090$
$S = 1.05$
2009 reflections
172 parameters
11 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.5412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ 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}
C1	0.2799 (3)	0.8073 (3)	0.9011 (2)	0.0165 (4)
C2	0.4454 (3)	0.7019 (3)	0.7727 (2)	0.0161 (4)
C3	0.5442 (3)	0.7791 (3)	0.6593 (2)	0.0172 (4)
H3	0.5097	0.8957	0.6633	0.021*
C4	0.6955 (3)	0.6798 (3)	0.5397 (2)	0.0168 (4)
C5	0.7464 (3)	0.5058 (3)	0.5320 (2)	0.0178 (4)
H5	0.8434	0.4414	0.4487	0.021*
C6	0.6522 (3)	0.4277 (3)	0.6494 (2)	0.0167 (4)
C7	0.5018 (3)	0.5267 (3)	0.7692 (2)	0.0178 (4)
H7	0.4382	0.4755	0.8476	0.021*
C8	0.8096 (3)	0.7607 (3)	0.4223 (2)	0.0178 (4)
Fe1	0.02840 (4)	0.88499 (4)	1.21504 (3)	0.01967 (14)
N1	0.7168 (3)	0.2480 (2)	0.6517 (2)	0.0204 (4)
H1A	0.7573	0.2077	0.5513	0.025*
H1B	0.6164	0.2203	0.6995	0.025*
O1	0.2198 (2)	0.7325 (2)	1.01815 (18)	0.0251 (4)
O2	0.2094 (2)	0.96615 (19)	0.88749 (19)	0.0208 (3)
O3	0.8199 (3)	0.8942 (2)	0.46223 (19)	0.0243 (4)
O4	0.8971 (2)	0.6932 (2)	0.28758 (18)	0.0252 (4)
O1W	0.0523 (3)	1.1127 (2)	1.2728 (2)	0.0341 (4)
H1W	0.112 (5)	1.105 (4)	1.340 (3)	0.051*
H2W	0.065 (5)	1.189 (3)	1.217 (3)	0.051*

O2W	0.0978 (4)	0.3865 (3)	0.1118 (3)	0.0480 (6)
H4W	0.074 (5)	0.464 (4)	0.177 (4)	0.072*
H3W	−0.001 (3)	0.401 (3)	0.078 (3)	0.072*
O3W	0.4365 (3)	0.1532 (3)	0.9066 (3)	0.0482 (6)
H5W	0.376 (5)	0.110 (5)	0.867 (5)	0.072*
H6W	0.360 (4)	0.231 (4)	0.972 (4)	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0130 (10)	0.0204 (11)	0.0149 (10)	−0.0057 (9)	−0.0015 (8)	−0.0024 (8)
C2	0.0146 (10)	0.0162 (11)	0.0146 (9)	−0.0043 (9)	−0.0008 (8)	0.0006 (8)
C3	0.0171 (10)	0.0140 (10)	0.0172 (10)	−0.0045 (8)	−0.0007 (8)	0.0008 (8)
C4	0.0159 (10)	0.0189 (11)	0.0144 (9)	−0.0070 (9)	−0.0015 (8)	0.0023 (8)
C5	0.0155 (10)	0.0177 (11)	0.0152 (10)	−0.0034 (9)	0.0014 (8)	−0.0031 (8)
C6	0.0167 (10)	0.0141 (10)	0.0180 (10)	−0.0047 (9)	−0.0040 (8)	0.0008 (8)
C7	0.0171 (10)	0.0172 (11)	0.0162 (10)	−0.0065 (9)	0.0003 (8)	0.0020 (8)
C8	0.0143 (10)	0.0189 (11)	0.0164 (10)	−0.0045 (9)	−0.0015 (8)	0.0046 (8)
Fe1	0.0206 (2)	0.0162 (2)	0.0187 (2)	−0.00647 (15)	0.00079 (13)	−0.00049 (12)
N1	0.0215 (10)	0.0140 (9)	0.0234 (9)	−0.0064 (8)	−0.0008 (7)	−0.0024 (7)
O1	0.0263 (9)	0.0215 (8)	0.0176 (8)	−0.0064 (7)	0.0075 (6)	0.0003 (6)
O2	0.0173 (8)	0.0148 (8)	0.0255 (8)	−0.0027 (6)	−0.0020 (6)	−0.0015 (6)
O3	0.0296 (9)	0.0217 (8)	0.0216 (8)	−0.0140 (7)	0.0013 (7)	0.0010 (6)
O4	0.0289 (9)	0.0252 (9)	0.0169 (8)	−0.0124 (8)	0.0065 (6)	−0.0010 (6)
O1W	0.0553 (13)	0.0231 (9)	0.0353 (10)	−0.0223 (9)	−0.0204 (9)	0.0055 (7)
O2W	0.0719 (16)	0.0267 (10)	0.0453 (12)	−0.0136 (11)	−0.0229 (11)	−0.0003 (9)
O3W	0.0409 (12)	0.0553 (15)	0.0587 (14)	−0.0314 (11)	−0.0048 (10)	−0.0085 (11)

Geometric parameters (Å, º)

C1—O1	1.254 (3)	C8—O3	1.262 (3)
C1—O2	1.262 (3)	Fe1—O1	2.1040 (16)
C1—C2	1.502 (3)	Fe1—O2^{i}	2.1364 (16)
C2—C3	1.392 (3)	Fe1—O1W	2.1458 (17)
C2—C7	1.393 (3)	Fe1—O4^{ii}	2.2387 (17)
C3—C4	1.392 (3)	Fe1—O3^{ii}	2.3416 (16)
C3—H3	0.9300	Fe1—N1^{iii}	2.376 (2)
C4—C5	1.390 (3)	N1—H1A	0.9000
C4—C8	1.499 (3)	N1—H1B	0.9000
C5—C6	1.396 (3)	O1W—H1W	0.815 (10)
C5—H5	0.9300	O1W—H2W	0.809 (9)
C6—C7	1.390 (3)	O2W—H4W	0.842 (10)
C6—N1	1.422 (3)	O2W—H3W	0.844 (10)
C7—H7	0.9300	O3W—H5W	0.843 (10)
C8—O4	1.256 (3)	O3W—H6W	0.840 (10)
O1—C1—O2	123.12 (19)	O1—Fe1—O4^{ii}	90.79 (6)
O1—C1—C2	118.08 (19)	O2^{i}—Fe1—O4^{ii}	89.97 (6)

O2—C1—C2	118.80 (18)	O1W—Fe1—O4^{ii}	148.03 (7)
C3—C2—C7	120.2 (2)	O1—Fe1—O3^{ii}	145.97 (6)
C3—C2—C1	119.97 (19)	O2^{i}—Fe1—O3^{ii}	91.37 (6)
C7—C2—C1	119.81 (19)	O1W—Fe1—O3^{ii}	90.96 (7)
C2—C3—C4	119.2 (2)	O4^{ii}—Fe1—O3^{ii}	57.10 (6)
C2—C3—H3	120.4	O1—Fe1—N1^{iii}	85.72 (7)
C4—C3—H3	120.4	O2^{i}—Fe1—N1^{iii}	172.50 (6)
C5—C4—C3	120.64 (19)	O1W—Fe1—N1^{iii}	83.48 (7)
C5—C4—C8	119.82 (19)	O4^{ii}—Fe1—N1^{iii}	94.39 (7)
C3—C4—C8	119.5 (2)	O3^{ii}—Fe1—N1^{iii}	85.91 (6)
C4—C5—C6	120.03 (19)	C6—N1—Fe1^{iii}	113.51 (14)
C4—C5—H5	120.0	C6—N1—H1A	108.9
C6—C5—H5	120.0	Fe1^{iii}—N1—H1A	108.9
C7—C6—C5	119.3 (2)	C6—N1—H1B	108.9
C7—C6—N1	120.25 (19)	Fe1^{iii}—N1—H1B	108.9
C5—C6—N1	120.36 (19)	H1A—N1—H1B	107.7
C6—C7—C2	120.5 (2)	C1—O1—Fe1	116.73 (14)
C6—C7—H7	119.7	C1—O2—Fe1^{i}	127.68 (14)
C2—C7—H7	119.7	C8—O3—Fe1^{iv}	88.55 (12)
O4—C8—O3	120.90 (19)	C8—O4—Fe1^{iv}	93.43 (13)
O4—C8—C4	119.9 (2)	Fe1—O1W—H1W	116 (2)
O3—C8—C4	119.15 (19)	Fe1—O1W—H2W	130 (2)
O1—Fe1—O2^{i}	100.34 (7)	H1W—O1W—H2W	105.6 (16)
O1—Fe1—O1W	120.69 (8)	H4W—O2W—H3W	110.9 (17)
O2^{i}—Fe1—O1W	89.59 (7)	H5W—O3W—H6W	111.2 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H3*W*···O2*W*^{v}	0.84 (1)	2.38 (1)	2.892 (5)	120 (1)
O3*W*—H5*W*···O2^{vi}	0.84 (1)	2.09 (2)	2.852 (3)	151 (4)
O3*W*—H6*W*···O2*W*^{vii}	0.84 (1)	2.07 (2)	2.865 (3)	157 (3)
O2*W*—H4*W*···O4^{viii}	0.84 (1)	2.05 (2)	2.816 (3)	151 (3)
O1*W*—H2*W*···O2*W*^{ix}	0.81 (1)	1.94 (1)	2.745 (3)	171 (3)
O1*W*—H1*W*···O3^{x}	0.82 (1)	1.91 (1)	2.705 (3)	163 (4)
N1—H1*B*···O3*W*	0.90	2.19	3.015 (3)	153

Symmetry codes: (v) $-x, -y+1, -z$; (vi) $x, y-1, z$; (vii) $x, y, z+1$; (viii) $x-1, y, z$; (ix) $x, y+1, z+1$; (x) $-x+1, -y+2, -z+2$.