metal-organic compounds

Tetraaquabis(2-{[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]sulfanyl}acetato)iron(II)

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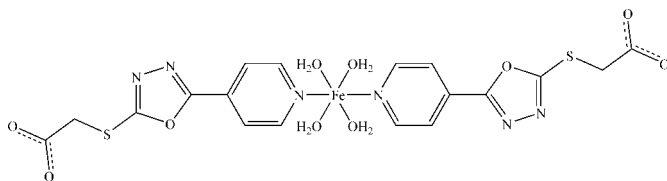
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In the title compound, $[Fe(C_9H_6N_3O_3S)_2(H_2O)_4]$ or $[Fe(POA)_2(H_2O)_4]$, the Fe^{II} atom is located on an inversion center and is ligated by four O atoms of coordinated water molecules in the equatorial plane while two POA ligands acting as monodentate ligands occupy the axial positions through their pyridyl N atoms, completing a slightly distorted octahedral coordination geometry. A three-dimensional supramolecular network is formed by multiple O—H⋯O hydrogen-bonding interactions between the coordinated water donors and the uncoordinated carboxyl acceptors.

Related literature

For the synthesis of 5-(4-pyridyl)-1,3,4-oxadiazole-2-thione, see: Young & Wood (1955). For metal-assisted transformation of *N*-benzoyldithiocarbazate to 5-phenyl-1,3,4-oxadiazole-2-thiol (pot) in the presence of ethylenediamine, and its first-row transition-metal complexes, see: Tripathi *et al.* (2007). For Zn^{II} and Cd^{II} metal-organic polymers with the versatile building block 5-(4-pyridyl)-1,3,4-oxadiazole-2-thiol, see: Du *et al.* (2006).

Experimental

Crystal data

$[Fe(C_9H_6N_3O_3S)_2(H_2O)_4]$	b = 10.709 (2) Å
M_r = 600.37	c = 7.5709 (15) Å
Monoclinic, $P2_1/c$	β = 91.45 (3)°
a = 14.365 (3) Å	V = 1164.2 (4) Å^3
Z = 2	T = 293 K
Mo $K\alpha$ radiation	$0.20 \times 0.20 \times 0.20$ mm
μ = 0.90 mm^{-1}	

Data collection

Siemens SMART CCD diffractometer	12366 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2285 independent reflections
T_{min} = 0.949, T_{max} = 1.000	2179 reflections with $I > 2\sigma(I)$
	R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.078	
S = 1.13	
2285 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
185 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—O1	2.0605 (17)	Fe1—N1	2.2359 (18)
Fe1—O2	2.1340 (18)		

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1A⋯O5^i	0.83 (3)	1.87 (3)	2.691 (3)	170 (3)
O1—H1B⋯O5^{ii}	0.83 (3)	1.82 (4)	2.649 (2)	174 (3)
O2—H2A⋯O4^{ii}	0.82 (3)	2.07 (3)	2.896 (3)	177 (3)
O2—H2B⋯O4^{iii}	0.84 (4)	1.98 (4)	2.817 (3)	175 (3)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); 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*.

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supporting information

Tetraaquabis(2-{[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]sulfanyl}acetato)iron(II)

Hai-Rong Wang and Guo-Ting Li

S1. Comment

Recently, pyridyl-containing 1,3,4-oxadiazole-2-thione have been systematically explored as promising bridging ligands in coordination chemistry. Metal- assisted transformation of *N*-benzoyldithiocarbazate to 5-phenyl-1,3,4-oxadiazole-2-thiol (pot) in the presence of ethylenediamine, and its first row transition metal complexes were discussed by N. K. Singh and coworkers [Tripathi *et al.*, (2007)]. A report describing Zn^{II} and Cd^{II} metal-organic polymers with a versatile building block 5-(4-pyridyl) -1,3,4-oxadiazole-2-thiol was presented by Du *et al.*, (2006). We purposedly engrafted the carboxylic group into the 5-(pyridin-4-yl)-1,3,4-oxadiazol-2-ylthio backbone and synthesized the multifunctional ligands 2-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-ylthio)acetic acid (HPOA). Herein we report that the reaction of FeSO$_4$.7H$_2$O and sodium(I) salt of HPOA leads to a new complex [Fe(POA)$_2$(H$_2$O)$_4$] (Fig.1).

The title compound is a mononuclear complex in which every Fe^{II} ion located at the inversion center *i* reproduces the whole molecule through the asymmetry unit consisting of one-half Fe^{II}, one deprotonated POA and two water molecules. In (1) the iron(II) center is ligated by four O from water molecules in the equatorial plane, and two POA anions acting as monodentate ligands and occupy the axial positions through their pyridyl nitrogen atoms coordinating to Fe^{II}, which is in an axial-elongated octahedral coordination sphere with the bond distances of Fe—O and Fe—N ranging from 2.0605 (17) to 2.2359 (18) Å (Table 1).

In (1) the uncoordinated carboxyl groups as typical hydrogen-bonding acceptors are authentically interesting in the construction of an intricate three-dimensional supramolecular network. Clearly, further aggregation of the monomers (1) is directed by the multiple hydrogen-bonding between the coordinated water donors and the uncoordinated carboxyl acceptors. Fig. 2 shows the complicated hydrogen-bonding system among monomers (1): each coordination water molecule in one monomer forms two O—H···O hydrogen bonds (Table 2) with carboxyl groups to bridge two monomers, while every carboxyl group of POA in the monomer acts as a three-connected hydrogen-bonding acceptor and adopts two different hydrogen-bonding models (bridging and chelating modes) to links with three monomers. Consequently, every monomer acts as a novel six-connected supramolecular synthon to connect with six adjacent monomers. In this way monomers (1) are arrayed to create a three-dimensional supramolecular architecture as shown in Fig. 3.

S2. Experimental

5-(4-pyridyl)-1,3,4-oxadiazole-2-thione was synthesized according to the reported method (Young & Wood, 1955). The sodium(I) salt of the ligand 2-(5-(pyridin-4-yl)-1,3,4-oxadiazol-2-ylthio)acetic acid (HPOA) was synthesized as the following process. To a solution of sodium hydroxide (1.60 g, 40 mmol) and 95% alcohol (50 ml) was added 5-pyridyl-2-mercapto-1,3,4-oxadiazole (3.58 g, 20 mmol) and the resulting mixture was refluxed for half an hour. And then a solution of chloroactic acid (1.89 g, 20 mmol) and 95% alcohol (70 ml) was dropwise added to the mixture with continuous refluxing for 3 h. Pale yellow precipitate was filtered. After recrystallized from alcohol/water (2:1), the obtained pure product was 2.76 g. Yield: 51%. Selected IR (cm^{-1}, KBr pellet): 3489(*w*), 1598(*s*), 1464(*m*), 1402(*s*), 1220(*m*), 1190(*m*),

1084(*m*), 909(*m*), 835(*m*), 704(w), 519(*m*).

The title compound (1), was prepared according to the following process. A mixture of NaPOA (51.8 mg, 0.2 mmol), FeSO$_4$.7H$_2$O (27.8 mg, 0.1 mmol) and deionized water (20 ml) was stirred for 30 minutes and then filtered. The filtrate was allowed to evaporate at room temperature for three days, and yellow crystals were obtain in 36% yield. Selected IR (cm^{-1}, KBr pellet): 3416(*m*), 3194(*m*), 1618(*s*), 1545(*s*), 1495(w), 1450(*s*), 1423(w), 1379(*s*), 1226(*m*), 1198(*m*), 1087(w), 1063(w), 1003(w), 871(w), 840(w), 799(w), 743(w), 707(*s*), 586(w), 522(w).

S3. Refinement

The H atoms of water molecules were located from difference Fourier maps, and their positional and isotropic displacement parameters were refined, while the other hydrogen atoms were assigned with common isotropic displacement factors [U_{iso}(H) = 1.2 times U_{eq}(C)] and included in the final refinement by using geometrical restraints.
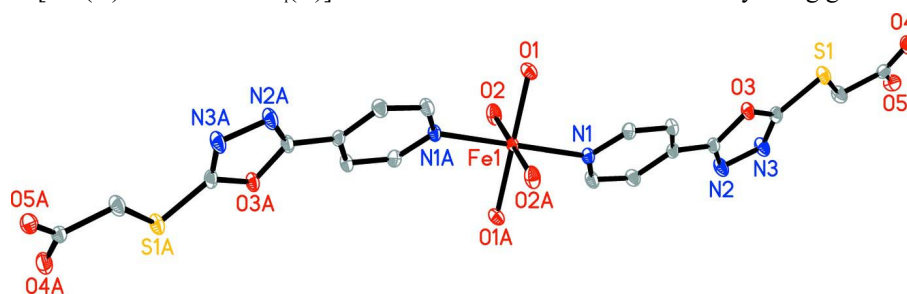

Figure 1

ORTEP diagram of (1) with atom numbering scheme showing coordination sphere of metal center Fe^{II} (30% probability ellipsoids for all non-hydrogen atoms). Symmetry code A: -*x*, -*y* + 1, -*z*.
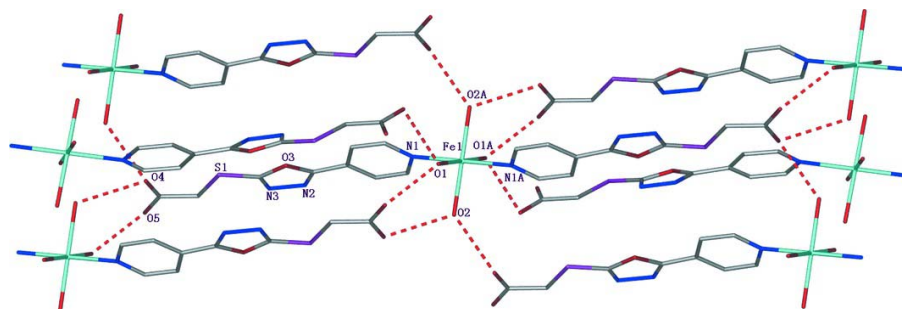

Figure 2

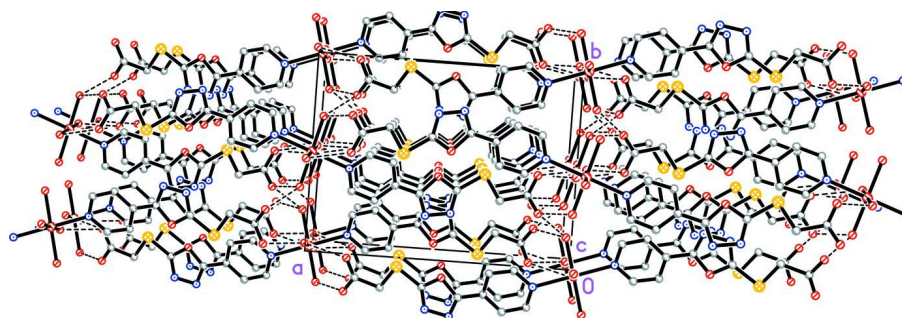View of a section of the hydrogen-bonding system among monomers (1).

Figure 3

View of three-dimensional hydrogen-bonding supramolecular network.

Tetraaquabis(2-{[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]sulfanyl}acetato) iron(II)

Crystal data

$[Fe(C_9H_6N_3O_3S)_2(H_2O)_4]$	$F(000) = 616$
$M_r = 600.37$	$D_x = 1.713$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3319 reflections
$a = 14.365$ (3) Å	$\theta = 2.4$–30.9°
$b = 10.709$ (2) Å	$\mu = 0.90$ mm^{-1}
$c = 7.5709$ (15) Å	$T = 293$ K
$\beta = 91.45$ (3)°	Prism, yellow
$V = 1164.2$ (4) Å^3	$0.20 \times 0.20 \times 0.20$ mm
$Z = 2$	

Data collection

Siemens SMART CCD diffractometer	12366 measured reflections
Radiation source: fine-focus sealed tube	2285 independent reflections
Graphite monochromator	2179 reflections with $I > 2\sigma(I)$
ω scan	$R_{int} = 0.034$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
	$h = -17 \rightarrow 17$
	$k = -13 \rightarrow 13$
$T_{min} = 0.949$, $T_{max} = 1.000$	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.036$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.078$	
$S = 1.13$	H atoms treated by a mixture of independent and constrained refinement
2285 reflections	
185 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2 + 0.5694P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.33$ e Å^{-3}
	$\Delta\rho_{min} = -0.25$ 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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Fe1	0.0000	0.5000	0.0000	0.02246 (14)

S1	0.65085 (4)	0.54011 (6)	0.38712 (8)	0.03380 (17)
O1	0.03673 (11)	0.31754 (16)	0.0529 (3)	0.0319 (4)
O2	−0.01063 (14)	0.52700 (19)	0.2780 (2)	0.0397 (5)
O3	0.48086 (10)	0.57082 (15)	0.2519 (2)	0.0302 (4)
O4	0.84192 (11)	0.52207 (17)	0.5162 (2)	0.0407 (4)
O5	0.84840 (11)	0.70106 (16)	0.6691 (2)	0.0397 (4)
N1	0.14562 (12)	0.57012 (18)	0.0402 (2)	0.0272 (4)
N2	0.44244 (13)	0.76466 (19)	0.3170 (3)	0.0381 (5)
N3	0.53408 (13)	0.74249 (19)	0.3821 (3)	0.0378 (5)
C1	0.21910 (15)	0.4960 (2)	0.0133 (3)	0.0281 (5)
H1	0.2093	0.4211	−0.0516	0.034*
C2	0.30836 (15)	0.5226 (2)	0.0746 (3)	0.0298 (5)
H2	0.3582	0.4665	0.0544	0.036*
C3	0.16251 (15)	0.6786 (2)	0.1237 (3)	0.0329 (5)
H3	0.1119	0.7341	0.1398	0.039*
C4	0.24920 (15)	0.7138 (2)	0.1873 (3)	0.0331 (5)
H4	0.2580	0.7920	0.2446	0.040*
C5	0.32349 (14)	0.6327 (2)	0.1658 (3)	0.0259 (5)
C6	0.41495 (14)	0.6630 (2)	0.2443 (3)	0.0277 (5)
C7	0.55192 (14)	0.6288 (2)	0.3411 (3)	0.0288 (5)
C8	0.70959 (16)	0.6582 (2)	0.5169 (3)	0.0367 (6)
H8A	0.7116	0.7366	0.4478	0.044*
H8B	0.6736	0.6747	0.6243	0.044*
C9	0.80811 (15)	0.6208 (2)	0.5712 (3)	0.0312 (5)
H2A	0.037 (2)	0.516 (3)	0.338 (4)	0.053 (9)*
H2B	−0.056 (3)	0.522 (3)	0.346 (5)	0.068 (11)*
H1A	0.067 (2)	0.281 (3)	−0.024 (4)	0.051 (9)*
H1B	0.070 (2)	0.312 (3)	0.145 (5)	0.066 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0168 (2)	0.0266 (2)	0.0237 (2)	0.00109 (17)	−0.00395 (17)	0.00006 (17)
S1	0.0217 (3)	0.0386 (3)	0.0406 (4)	0.0032 (2)	−0.0081 (2)	−0.0074 (3)
O1	0.0271 (9)	0.0336 (9)	0.0345 (10)	0.0056 (7)	−0.0080 (8)	0.0003 (8)
O2	0.0267 (9)	0.0674 (13)	0.0250 (9)	0.0050 (9)	−0.0024 (8)	−0.0034 (8)
O3	0.0180 (8)	0.0341 (9)	0.0380 (9)	−0.0009 (6)	−0.0067 (7)	−0.0049 (7)
O4	0.0249 (9)	0.0502 (11)	0.0468 (11)	0.0041 (8)	−0.0009 (8)	0.0008 (9)
O5	0.0322 (9)	0.0462 (10)	0.0399 (10)	−0.0095 (8)	−0.0174 (8)	0.0072 (8)
N1	0.0174 (9)	0.0328 (11)	0.0311 (10)	−0.0016 (8)	−0.0037 (8)	0.0004 (8)
N2	0.0216 (10)	0.0379 (12)	0.0539 (13)	0.0011 (8)	−0.0125 (9)	−0.0074 (10)
N3	0.0223 (10)	0.0368 (12)	0.0536 (13)	0.0004 (8)	−0.0136 (9)	−0.0090 (10)
C1	0.0229 (11)	0.0314 (12)	0.0298 (11)	−0.0027 (9)	−0.0001 (9)	−0.0026 (9)
C2	0.0191 (11)	0.0351 (13)	0.0352 (12)	0.0029 (9)	−0.0010 (9)	−0.0024 (10)
C3	0.0209 (11)	0.0311 (12)	0.0464 (14)	0.0024 (9)	−0.0052 (10)	−0.0042 (11)
C4	0.0267 (12)	0.0297 (12)	0.0425 (14)	−0.0005 (10)	−0.0043 (10)	−0.0050 (10)
C5	0.0176 (10)	0.0337 (12)	0.0262 (11)	−0.0044 (9)	−0.0036 (9)	0.0042 (9)
C6	0.0177 (10)	0.0338 (13)	0.0315 (12)	0.0011 (9)	−0.0012 (9)	0.0009 (10)

C7	0.0184 (10)	0.0376 (13)	0.0302 (12)	−0.0044 (9)	−0.0041 (9)	−0.0014 (10)
C8	0.0270 (12)	0.0391 (14)	0.0433 (14)	−0.0001 (10)	−0.0134 (11)	−0.0039 (11)
C9	0.0230 (11)	0.0401 (14)	0.0303 (12)	−0.0037 (10)	−0.0028 (9)	0.0108 (11)

Geometric parameters (Å, º)

Fe1—O1^i	2.0605 (17)	N1—C3	1.341 (3)
Fe1—O1	2.0605 (17)	N2—C6	1.278 (3)
Fe1—O2	2.1340 (18)	N2—N3	1.414 (3)
Fe1—O2^i	2.1340 (18)	N3—C7	1.284 (3)
Fe1—N1^i	2.2359 (18)	C1—C2	1.382 (3)
Fe1—N1	2.2359 (18)	C1—H1	0.9500
S1—C7	1.737 (2)	C2—C5	1.381 (3)
S1—C8	1.799 (2)	C2—H2	0.9500
O1—H1A	0.83 (3)	C3—C4	1.377 (3)
O1—H1B	0.83 (3)	C3—H3	0.9500
O2—H2A	0.82 (3)	C4—C5	1.389 (3)
O2—H2B	0.84 (4)	C4—H4	0.9500
O3—C7	1.360 (2)	C5—C6	1.464 (3)
O3—C6	1.368 (3)	C8—C9	1.517 (3)
O4—C9	1.240 (3)	C8—H8A	0.9900
O5—C9	1.265 (3)	C8—H8B	0.9900
N1—C1	1.340 (3)		
O1^i—Fe1—O1	180.0	N1—C1—H1	118.2
O1^i—Fe1—O2	92.22 (8)	C2—C1—H1	118.2
O1—Fe1—O2	87.78 (8)	C5—C2—C1	118.5 (2)
O1^i—Fe1—O2^i	87.78 (8)	C5—C2—H2	120.8
O1—Fe1—O2^i	92.22 (8)	C1—C2—H2	120.8
O2—Fe1—O2^i	180.00 (11)	N1—C3—C4	123.6 (2)
O1^i—Fe1—N1^i	93.33 (7)	N1—C3—H3	118.2
O1—Fe1—N1^i	86.67 (7)	C4—C3—H3	118.2
O2—Fe1—N1^i	95.14 (8)	C3—C4—C5	118.6 (2)
O2^i—Fe1—N1^i	84.86 (8)	C3—C4—H4	120.7
O1^i—Fe1—N1	86.67 (7)	C5—C4—H4	120.7
O1—Fe1—N1	93.33 (7)	C2—C5—C4	118.74 (19)
O2—Fe1—N1	84.86 (8)	C2—C5—C6	121.4 (2)
O2^i—Fe1—N1	95.14 (8)	C4—C5—C6	119.9 (2)
N1^i—Fe1—N1	180.0	N2—C6—O3	112.99 (18)
C7—S1—C8	95.46 (11)	N2—C6—C5	128.9 (2)
Fe1—O1—H1A	116 (2)	O3—C6—C5	118.03 (19)
Fe1—O1—H1B	112 (2)	N3—C7—O3	113.64 (19)
H1A—O1—H1B	105 (3)	N3—C7—S1	129.59 (17)
Fe1—O2—H2A	116 (2)	O3—C7—S1	116.75 (17)
Fe1—O2—H2B	132 (2)	C9—C8—S1	112.55 (17)
H2A—O2—H2B	108 (3)	C9—C8—H8A	109.1
C7—O3—C6	101.62 (17)	S1—C8—H8A	109.1
C1—N1—C3	116.77 (19)	C9—C8—H8B	109.1

C1—N1—Fe1	121.21 (15)	S1—C8—H8B	109.1
C3—N1—Fe1	120.82 (15)	H8A—C8—H8B	107.8
C6—N2—N3	106.39 (19)	O4—C9—O5	126.8 (2)
C7—N3—N2	105.35 (18)	O4—C9—C8	120.3 (2)
N1—C1—C2	123.7 (2)	O5—C9—C8	112.9 (2)
O1^i—Fe1—N1—C1	−152.98 (18)	C3—C4—C5—C2	2.9 (3)
O1—Fe1—N1—C1	27.02 (18)	C3—C4—C5—C6	−175.1 (2)
O2—Fe1—N1—C1	114.48 (18)	N3—N2—C6—O3	−0.5 (3)
O2^i—Fe1—N1—C1	−65.52 (18)	N3—N2—C6—C5	175.9 (2)
N1^i—Fe1—N1—C1	7 (44)	C7—O3—C6—N2	0.8 (3)
O1^i—Fe1—N1—C3	39.94 (18)	C7—O3—C6—C5	−176.01 (19)
O1—Fe1—N1—C3	−140.06 (18)	C2—C5—C6—N2	172.6 (2)
O2—Fe1—N1—C3	−52.59 (18)	C4—C5—C6—N2	−9.4 (4)
O2^i—Fe1—N1—C3	127.41 (18)	C2—C5—C6—O3	−11.1 (3)
N1^i—Fe1—N1—C3	−161 (44)	C4—C5—C6—O3	166.9 (2)
C6—N2—N3—C7	0.0 (3)	N2—N3—C7—O3	0.6 (3)
C3—N1—C1—C2	3.6 (3)	N2—N3—C7—S1	−177.87 (18)
Fe1—N1—C1—C2	−164.01 (18)	C6—O3—C7—N3	−0.8 (3)
N1—C1—C2—C5	−1.3 (4)	C6—O3—C7—S1	177.81 (15)
C1—N1—C3—C4	−2.6 (3)	C8—S1—C7—N3	3.4 (3)
Fe1—N1—C3—C4	165.05 (19)	C8—S1—C7—O3	−174.96 (18)
N1—C3—C4—C5	−0.6 (4)	C7—S1—C8—C9	−174.28 (18)
C1—C2—C5—C4	−2.0 (3)	S1—C8—C9—O4	4.8 (3)
C1—C2—C5—C6	176.0 (2)	S1—C8—C9—O5	−177.06 (17)

Symmetry code: (i) −x, −y+1, −z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O5^{ii}	0.83 (3)	1.87 (3)	2.691 (3)	170 (3)
O1—H1B···O5^{iii}	0.83 (3)	1.82 (4)	2.649 (2)	174 (3)
O2—H2A···O4^{iii}	0.82 (3)	2.07 (3)	2.896 (3)	177 (3)
O2—H2B···O4^{iv}	0.84 (4)	1.98 (4)	2.817 (3)	175 (3)

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