

Tetraaquabis(2-[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]sulfanyl)acetatoiron(II)

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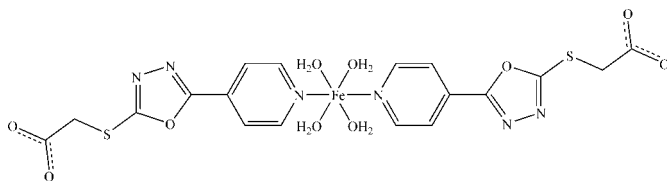
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.078; data-to-parameter ratio = 12.4.

In the title compound, $[\text{Fe}(\text{C}_9\text{H}_6\text{N}_3\text{O}_3\text{S})_2(\text{H}_2\text{O})_4]$ or $[\text{Fe}(\text{POA})_2(\text{H}_2\text{O})_4]$, 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 $\text{O}-\text{H}\cdots\text{O}$ 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*-benzoyldithiocarbamate 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

$[\text{Fe}(\text{C}_9\text{H}_6\text{N}_3\text{O}_3\text{S})_2(\text{H}_2\text{O})_4]$
 $M_r = 600.37$
 Monoclinic, $P2_1/c$
 $a = 14.365$ (3) Å

$b = 10.709$ (2) Å
 $c = 7.5709$ (15) Å
 $\beta = 91.45$ (3)°
 $V = 1164.2$ (4) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.90$ mm⁻¹

$T = 293$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Siemens SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.949$, $T_{\text{max}} = 1.000$

12366 measured reflections
 2285 independent reflections
 2179 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.078$
 $S = 1.13$
 2285 reflections
 185 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ 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, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O5 ⁱ	0.83 (3)	1.87 (3)	2.691 (3)	170 (3)
O1—H1B \cdots O5 ⁱⁱ	0.83 (3)	1.82 (4)	2.649 (2)	174 (3)
O2—H2A \cdots O4 ⁱⁱ	0.82 (3)	2.07 (3)	2.896 (3)	177 (3)
O2—H2B \cdots 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2366).

References

- Du, M., Zhang, Z. H., Zhao, X.-J. & Xu, Q. (2006). *Inorg. Chem.* **45**, 5785–5792.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Siemens (1994). SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Siemens (1996). SMART. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Tripathi, P., Pal, A., Jancik, V., Pandey, A. K., Singh, J. & Singh, N. K. (2007). *Polyhedron*, **26**, 2597–2602.
- Young, R. W. & Wood, K. H. (1955). *J. Am. Chem. Soc.* **77**, 400–403.

supplementary materials

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

H.-R. Wang and G.-T. Li

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*-benzoyldithiocarbamate 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 purposely 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 FeSO₄·7H₂O and sodium(I) salt of HPOA leads to a new complex [Fe(POA)₂(H₂O)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.

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 chloroacetic 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

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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), $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ (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 obtained 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).

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 [$U_{\text{iso}}(\text{H}) = 1.2 \text{ times } U_{\text{eq}}(\text{C})$] and included in the final refinement by using geometrical restraints.

Figures

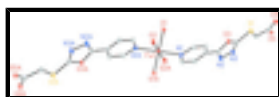


Fig. 1. ORTEP diagram of (1) with atom numbering scheme showing coordination sphere of metal center Fe^{II} (30% probability ellipsoids for all non-hydrogen atoms). Symmetry code A: $-x, -y + 1, -z$.

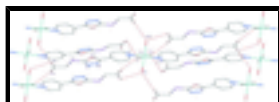


Fig. 2. View of a section of the hydrogen-bonding system among monomers (1).

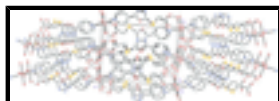


Fig. 3. View of three-dimensional hydrogen-bonding supramolecular network.

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

Crystal data

$[\text{Fe}(\text{C}_9\text{H}_6\text{N}_3\text{O}_3\text{S})_2(\text{H}_2\text{O})_4]$

$M_r = 600.37$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 14.365\ (3)\ \text{\AA}$

$b = 10.709\ (2)\ \text{\AA}$

$c = 7.5709\ (15)\ \text{\AA}$

$\beta = 91.45\ (3)^\circ$

$V = 1164.2\ (4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 616$

$D_x = 1.713\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3319 reflections

$\theta = 2.4\text{--}30.9^\circ$

$\mu = 0.90\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, yellow

$0.20 \times 0.20 \times 0.20\ \text{mm}$

Data collection

Siemens SMART CCD

2285 independent reflections

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

Refinement

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

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	0.0000	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)

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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 (\AA^2)

	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 (\AA , $^\circ$)

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)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O5 ⁱⁱ	0.83 (3)	1.87 (3)	2.691 (3)	170 (3)
O1—H1B \cdots O5 ⁱⁱⁱ	0.83 (3)	1.82 (4)	2.649 (2)	174 (3)
O2—H2A \cdots O4 ⁱⁱⁱ	0.82 (3)	2.07 (3)	2.896 (3)	177 (3)
O2—H2B \cdots 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) $x-1, y, z$.

Fig. 1

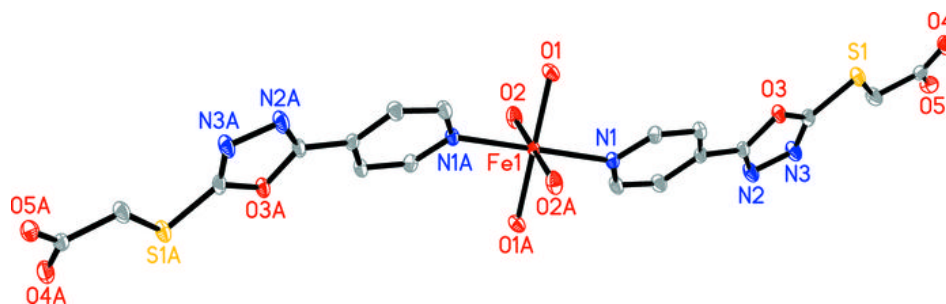


Fig. 2

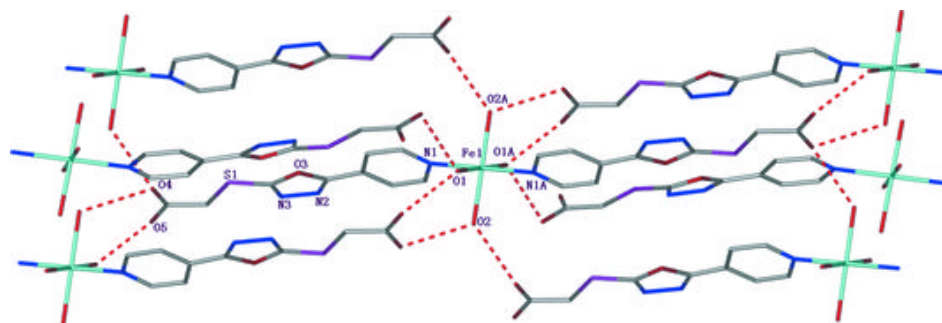


Fig. 3

