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2,9-Dimethyl-1,10-phenanthrolinium bis(pyridine-2,6-dicarboxylato-κ^3O,N,O')ferrate(III) dihydrate

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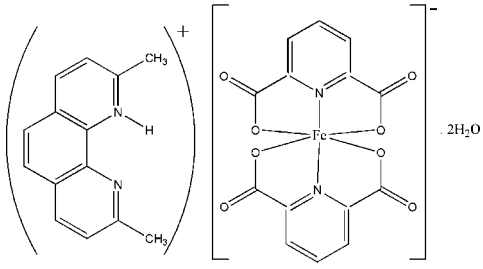
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.165; data-to-parameter ratio = 15.3.

The title compound, $(C_{14}H_{13}N_2)[Fe(C_7H_3NO_4)_2]\cdot 2H_2O$ or (dmpH)[Fe(pydc)$_2$]·2H$_2$O (dmp is 2,9-dimethyl-1,10-phenanthroline and pydcH$_2$ is pyridine-2,6-dicarboxylic acid), is a six-coordinate Fe^{III} complex obtained by reacting neocuproine (dmp), dipicolinic acid (pydcH$_2$) and iron(II) chloride. The anionic six-coordinate complex has a distorted octahedral geometry and is connected to its counter-cation by a number of intermolecular interactions, forming infinite one-dimensional chains in the [010] direction. Ion pairing, metal–ligand coordination and van der Waals forces, as well as intermolecular X—H···O hydrogen bonds (X = O, N and C) and π–π stacking interactions [with centroid-to-centroid separations of 3.531 and 3.457 Å, shortest interplanar distances of 3.355 and 3.449 Å, and interplanar angles of 1.89 and 5.45°], result in a three-dimensional framework.

Related literature

There are several reports on proton transfer between a carboxylic acid and a heterocyclic amine, and on the ability of the resulting self-associated proton-transfer systems to react with metal ions, affording transition metal complexes (Aghabozorg *et al.*, 2006; Zhao *et al.*, 2005).



Experimental

Crystal data

$(C_{14}H_{13}N_2)[Fe(C_7H_3NO_4)_2]\cdot 2H_2O$
M_r = 631.35
Monoclinic, $P2_1/n$
a = 8.9535 (14) Å
b = 18.607 (3) Å
c = 15.674 (2) Å
β = 94.826 (3)°
V = 2602.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 150 (2) K
0.50 × 0.40 × 0.08 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.737, T_{max} = 0.950
29654 measured reflections
5986 independent reflections
2776 reflections with $I > 2\sigma(I)$
R_{int} = 0.127

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.165
S = 0.89
5986 reflections
390 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9B···O10^{i}	0.95	2.01	2.907 (5)	157
O9—H9A···O5	0.95	1.99	2.866 (4)	153
O10—H10A···O7^{ii}	0.95	2.11	2.964 (4)	150
C3—H3···O7^{iii}	0.95	2.45	3.304 (5)	150
C12—H12···O2^{iv}	0.95	2.39	3.263 (5)	152
C17—H17···O9^{iv}	0.95	2.41	3.357 (5)	175

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: BH2100).

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supplementary materials

Acta Cryst. (2007). E**63**, m1760 [**doi:10.1107/S1600536807025081**]

2,9-Dimethyl-1,10-phenanthrolinium bis(pyridine-2,6-dicarboxylato-κ^3O,N,O')ferrate(III) dihydrate

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Comment

Continuing our research on proton-transfer compounds, we reached a system which is highly soluble in polar solvents. This compound has not been crystallized until now, but its metal-organic derivatives can be obtained as suitable crystals. In this report, the crystal structure of the iron(III) derivative is described.

The Fe^{III} ion is located at the centre of a distorted octahedral arrangement (Fig. 1). The O1—Fe1—O5—C8 [92.4 (3)°], O1—Fe1—O8—C14 [−91.4 (3)°], O8—Fe1—O1—C1 [−96.6 (3)°] and O8—Fe1—O4—C7 [98.1 (3)°] torsion angles, and O1—Fe1—O8 [95.78 (12)°] and O4—Fe1—O5 [94.88 (11)°] bond angles indicate that the dianionic $pydc^{2-}$ units are almost perpendicular to each other. The important characteristic of the crystal structure is the infinite one dimensional chains based on [010] vector. Figure 2 shows the wavy chains of $[Fe(pydc)_2]^-$ complex anions formed through the C—H···O interactions, in which the $R_2^2(10)$ and $C_2^2(16)$ graph set can be observed. The space between two chains is filled with $dmpH^+$ cations and lattice water molecules. Hydrogen bonds play an important role in stabilizing the crystal structure.

Other intermolecular interactions exist between aromatic cations and the ligands bonded to the metal center. The centroid to centroid separation between the π–systems of the cation, labeled as B, and the anion, A1 and A2, are 3.531 and 3.457 Å, respectively (Fig. 3). The shortest interplanar distances for A1/B (3.355 Å) and A2/B (3.449 Å) and their related interplanar angles, 1.89 and 5.45°, respectively, confirm the effective π–π stacking interactions. Therefore, in the formation of this Fe^{III} complex, ion pairing, metal–ligand coordinations, hydrogen–bonding and π–π stacking as well as van der Waals forces, play important roles in the construction of the observed three–dimensional network.

Experimental

A solution of $FeCl_2$ (50 mg, 0.25 mmol) in water (10 ml) was added to 10 ml of an aqueous solution of dmp (105 mg, 0.5 mmol) and $pydcH_2$ (69 mg, 0.5 mmol). Pale yellow crystals of the title compound were obtained after allowing the mixture to stand for a week at room temperature.

Refinement

C and N-bonded H atoms were positioned geometrically and refined using a riding model (including torsional freedom for methyl groups), with C—H = 0.95–0.98 Å, and with U_{iso}(H) constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. H atoms for water molecules were found in a difference map and their parameters constrained to fit an idealized geometry: O—H = 0.95 Å and U_{iso}(H) = 1.2U_{iso}(carrier O).

Figures

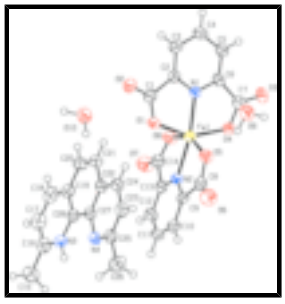


Fig. 1. The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level.

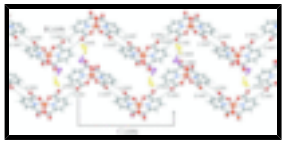


Fig. 2. A view of the chains formed by C—H···O interactions; water molecules (yellow and purple) are located in the space between chains and connected *via* O—H···O hydrogen bonds; $dmpH^+$ cations are omitted for clarity.

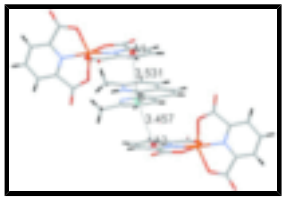


Fig. 3. Representation of separations between cation and anions.

2,9-Dimethyl-1,10-phenanthrolinium bis(pyridine-2,6-dicarboxylato-κ^3*O*,*N*,*O*')ferrate(III) dihydrate

Crystal data

$(C_{14}H_{13}N_2)[Fe(C_7H_3N_1O_4)_2]\cdot 2H_2O$	F_{000} = 1300
M_r = 631.35	D_x = 1.612 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3591 reflections
a = 8.9535 (14) Å	θ = 2.5–25.3º
b = 18.607 (3) Å	μ = 0.65 mm^{-1}
c = 15.674 (2) Å	T = 150 (2) K
β = 94.826 (3)º	Plate, pale yellow
V = 2602.1 (7) Å^3	0.50 × 0.40 × 0.08 mm
Z = 4	

Data collection

Bruker SMART diffractometer	5986 independent reflections
Radiation source: fine-focus sealed tube	2776 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.127
Detector resolution: 100 pixels mm^{-1}	θ_{max} = 27.7º
T = 150(2) K	θ_{min} = 1.7º
ω scans	h = −11→11

Absorption correction: multi-scan (SADABS; Sheldrick, 1998)

T_{min} = 0.737, T_{max} = 0.950

29654 measured reflections

k = −24→23

l = −20→20

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.058

$wR(F^2)$ = 0.165

S = 0.89

5986 reflections

390 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.55 e Å^{-3}

$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.00816 (6)	0.59166 (3)	0.79981 (3)	0.03083 (19)
N1	0.0103 (3)	0.59937 (17)	0.66923 (19)	0.0271 (7)
N2	0.0118 (3)	0.60327 (17)	0.93011 (19)	0.0290 (8)
N3	0.1130 (3)	0.85237 (17)	1.1817 (2)	0.0308 (8)
H3A	0.1723	0.8278	1.2255	0.037*
N4	0.3022 (3)	0.74239 (18)	1.1490 (2)	0.0337 (8)
O1	0.1666 (3)	0.66723 (15)	0.78243 (16)	0.0374 (7)
O2	0.2907 (3)	0.72973 (16)	0.68816 (17)	0.0453 (8)
O3	−0.2573 (3)	0.46501 (16)	0.63913 (18)	0.0467 (8)
O4	−0.1384 (3)	0.51698 (14)	0.75482 (16)	0.0351 (7)
O5	0.1630 (3)	0.52142 (15)	0.84458 (17)	0.0382 (7)
O6	0.2980 (3)	0.47772 (17)	0.9602 (2)	0.0555 (9)
O7	−0.2787 (3)	0.72774 (17)	0.91050 (18)	0.0516 (9)
O8	−0.1594 (3)	0.66250 (15)	0.81730 (16)	0.0390 (7)
O9	0.1840 (3)	0.43660 (17)	0.69343 (19)	0.0573 (9)
H9B	0.1065	0.4021	0.6964	0.069*
H9A	0.1900	0.4509	0.7518	0.069*
O10	0.4860 (3)	0.80382 (17)	0.80094 (18)	0.0598 (9)
H10B	0.5093	0.8536	0.8009	0.072*
H10A	0.5375	0.7847	0.8514	0.072*
C1	0.1945 (4)	0.6862 (2)	0.7062 (3)	0.0352 (10)
C2	0.0991 (4)	0.6478 (2)	0.6361 (2)	0.0295 (9)
C3	0.0992 (4)	0.6569 (2)	0.5490 (2)	0.0361 (10)
H3	0.1638	0.6907	0.5256	0.043*
C4	0.0022 (4)	0.6152 (2)	0.4967 (3)	0.0377 (10)
H4	−0.0015	0.6203	0.4363	0.045*

C5	−0.0902 (4)	0.5654 (2)	0.5332 (3)	0.0349 (10)
H5	−0.1581	0.5368	0.4979	0.042*
C6	−0.0822 (4)	0.5584 (2)	0.6199 (2)	0.0294 (9)
C7	−0.1676 (4)	0.5071 (2)	0.6735 (3)	0.0335 (10)
C8	0.2013 (4)	0.5167 (2)	0.9265 (3)	0.0356 (10)
C9	0.1112 (4)	0.5660 (2)	0.9794 (3)	0.0311 (9)
C10	0.1242 (5)	0.5746 (2)	1.0666 (3)	0.0384 (11)
H10	0.1962	0.5482	1.1020	0.046*
C11	0.0282 (5)	0.6232 (2)	1.1014 (3)	0.0416 (11)
H11	0.0336	0.6296	1.1617	0.050*
C12	−0.0744 (5)	0.6620 (2)	1.0500 (2)	0.0382 (11)
H12	−0.1390	0.6956	1.0739	0.046*
C13	−0.0806 (4)	0.6508 (2)	0.9628 (2)	0.0328 (10)
C14	−0.1835 (4)	0.6849 (2)	0.8936 (3)	0.0357 (10)
C15	0.0199 (5)	0.9230 (3)	1.2958 (3)	0.0496 (13)
H15C	0.0366	0.8793	1.3304	0.074*
H15B	−0.0775	0.9438	1.3062	0.074*
H15A	0.0994	0.9578	1.3118	0.074*
C16	0.0215 (4)	0.9047 (2)	1.2041 (3)	0.0404 (11)
C17	−0.0667 (5)	0.9402 (2)	1.1396 (3)	0.0454 (12)
H17	−0.1329	0.9774	1.1539	0.054*
C18	−0.0577 (4)	0.9213 (2)	1.0562 (3)	0.0457 (12)
H18	−0.1187	0.9456	1.0128	0.055*
C19	0.0387 (4)	0.8672 (2)	1.0329 (3)	0.0359 (10)
C20	0.0586 (5)	0.8467 (2)	0.9465 (3)	0.0442 (11)
H20	0.0003	0.8696	0.9009	0.053*
C21	0.1576 (5)	0.7959 (2)	0.9285 (3)	0.0428 (11)
H21	0.1706	0.7845	0.8705	0.051*
C22	0.2434 (4)	0.7591 (2)	0.9956 (3)	0.0358 (10)
C23	0.3494 (5)	0.7056 (2)	0.9805 (3)	0.0397 (11)
H23	0.3669	0.6928	0.9235	0.048*
C24	0.4261 (5)	0.6725 (2)	1.0473 (3)	0.0429 (11)
H24	0.4982	0.6367	1.0373	0.052*
C25	0.3988 (4)	0.6913 (2)	1.1322 (3)	0.0390 (11)
C26	0.4740 (5)	0.6527 (3)	1.2077 (3)	0.0553 (13)
H26C	0.4998	0.6871	1.2539	0.083*
H26B	0.5655	0.6295	1.1911	0.083*
H26A	0.4061	0.6162	1.2275	0.083*
C27	0.2274 (4)	0.7761 (2)	1.0811 (2)	0.0323 (9)
C28	0.1244 (4)	0.8313 (2)	1.0993 (2)	0.0321 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0346 (3)	0.0349 (4)	0.0232 (3)	−0.0007 (3)	0.0037 (2)	−0.0011 (3)
N1	0.0287 (17)	0.0283 (19)	0.0244 (16)	0.0021 (15)	0.0027 (13)	−0.0016 (15)
N2	0.0318 (18)	0.032 (2)	0.0233 (17)	−0.0043 (15)	0.0002 (14)	−0.0010 (15)
N3	0.0239 (17)	0.036 (2)	0.0317 (19)	−0.0033 (15)	−0.0006 (14)	0.0042 (16)

N4	0.0345 (19)	0.034 (2)	0.0315 (19)	−0.0059 (16)	−0.0070 (15)	−0.0004 (16)
O1	0.0468 (17)	0.0402 (18)	0.0247 (15)	−0.0065 (14)	−0.0004 (12)	−0.0026 (13)
O2	0.0473 (18)	0.046 (2)	0.0425 (18)	−0.0196 (16)	0.0046 (14)	0.0031 (15)
O3	0.0488 (19)	0.044 (2)	0.0463 (19)	−0.0172 (16)	−0.0025 (15)	−0.0075 (16)
O4	0.0382 (16)	0.0403 (18)	0.0271 (15)	−0.0050 (13)	0.0042 (12)	0.0022 (13)
O5	0.0404 (17)	0.0379 (18)	0.0368 (17)	0.0023 (14)	0.0058 (13)	−0.0042 (14)
O6	0.053 (2)	0.052 (2)	0.059 (2)	0.0143 (17)	−0.0112 (16)	0.0048 (17)
O7	0.0519 (19)	0.054 (2)	0.049 (2)	0.0192 (17)	0.0067 (15)	−0.0050 (17)
O8	0.0437 (17)	0.0455 (19)	0.0271 (16)	0.0076 (14)	−0.0010 (13)	−0.0008 (14)
O9	0.069 (2)	0.054 (2)	0.050 (2)	−0.0097 (18)	0.0111 (17)	−0.0099 (17)
O10	0.084 (3)	0.042 (2)	0.050 (2)	0.0052 (18)	−0.0086 (18)	−0.0004 (17)
C1	0.035 (2)	0.031 (3)	0.039 (3)	0.004 (2)	0.0014 (19)	0.003 (2)
C2	0.029 (2)	0.029 (2)	0.031 (2)	0.0010 (18)	0.0052 (17)	0.0006 (19)
C3	0.040 (2)	0.036 (3)	0.034 (2)	0.002 (2)	0.0096 (19)	0.008 (2)
C4	0.047 (3)	0.040 (3)	0.026 (2)	0.010 (2)	0.0002 (19)	0.000 (2)
C5	0.038 (2)	0.031 (2)	0.035 (2)	0.0081 (19)	−0.0026 (19)	−0.005 (2)
C6	0.028 (2)	0.028 (2)	0.032 (2)	0.0048 (18)	0.0011 (17)	−0.0052 (19)
C7	0.034 (2)	0.034 (3)	0.033 (2)	0.005 (2)	0.0022 (18)	0.000 (2)
C8	0.031 (2)	0.035 (3)	0.040 (3)	−0.008 (2)	0.0027 (19)	0.000 (2)
C9	0.034 (2)	0.029 (2)	0.031 (2)	−0.0057 (18)	0.0021 (18)	0.0056 (19)
C10	0.043 (3)	0.041 (3)	0.030 (2)	−0.015 (2)	−0.0042 (19)	0.006 (2)
C11	0.056 (3)	0.047 (3)	0.021 (2)	−0.021 (2)	0.002 (2)	−0.003 (2)
C12	0.044 (3)	0.040 (3)	0.032 (2)	−0.008 (2)	0.007 (2)	−0.010 (2)
C13	0.034 (2)	0.033 (3)	0.032 (2)	−0.0094 (19)	0.0051 (18)	−0.001 (2)
C14	0.037 (2)	0.034 (3)	0.036 (3)	0.002 (2)	0.0032 (19)	−0.001 (2)
C15	0.041 (3)	0.060 (3)	0.049 (3)	0.003 (2)	0.015 (2)	−0.011 (3)
C16	0.027 (2)	0.045 (3)	0.050 (3)	−0.006 (2)	0.008 (2)	−0.003 (2)
C17	0.029 (2)	0.044 (3)	0.063 (3)	0.002 (2)	0.005 (2)	0.000 (3)
C18	0.030 (2)	0.044 (3)	0.062 (3)	0.000 (2)	−0.004 (2)	0.012 (3)
C19	0.028 (2)	0.036 (3)	0.043 (3)	−0.0035 (19)	−0.0033 (18)	0.006 (2)
C20	0.053 (3)	0.045 (3)	0.032 (3)	−0.001 (2)	−0.013 (2)	0.007 (2)
C21	0.058 (3)	0.041 (3)	0.029 (2)	−0.007 (2)	−0.002 (2)	0.002 (2)
C22	0.040 (2)	0.034 (3)	0.034 (2)	−0.010 (2)	0.0036 (19)	−0.003 (2)
C23	0.046 (3)	0.039 (3)	0.035 (3)	−0.010 (2)	0.009 (2)	−0.004 (2)
C24	0.044 (3)	0.034 (3)	0.051 (3)	−0.002 (2)	0.008 (2)	−0.004 (2)
C25	0.036 (2)	0.035 (3)	0.044 (3)	−0.005 (2)	−0.006 (2)	0.001 (2)
C26	0.062 (3)	0.045 (3)	0.057 (3)	0.009 (3)	−0.007 (2)	0.004 (3)
C27	0.030 (2)	0.031 (2)	0.035 (2)	−0.0062 (19)	0.0004 (17)	−0.001 (2)
C28	0.030 (2)	0.034 (3)	0.032 (2)	−0.0071 (19)	0.0009 (17)	0.0021 (19)

Geometric parameters (Å, °)

Fe1—O5	1.990 (3)	C8—C9	1.514 (5)
Fe1—O4	1.999 (3)	C9—C10	1.371 (5)
Fe1—O1	2.032 (3)	C10—C11	1.390 (6)
Fe1—O8	2.033 (3)	C10—H10	0.9500
Fe1—N2	2.051 (3)	C11—C12	1.375 (5)
Fe1—N1	2.054 (3)	C11—H11	0.9500
N1—C6	1.325 (5)	C12—C13	1.379 (5)

N1—C2	1.335 (4)	C12—H12	0.9500
N2—C9	1.325 (5)	C13—C14	1.503 (5)
N2—C13	1.342 (5)	C15—C16	1.479 (5)
N3—C16	1.338 (5)	C15—H15C	0.9800
N3—C28	1.362 (5)	C15—H15B	0.9800
N3—H3A	0.9501	C15—H15A	0.9800
N4—C25	1.326 (5)	C16—C17	1.395 (6)
N4—C27	1.362 (5)	C17—C18	1.363 (6)
O1—C1	1.290 (4)	C17—H17	0.9500
O2—C1	1.232 (5)	C18—C19	1.395 (6)
O3—C7	1.216 (4)	C18—H18	0.9500
O4—C7	1.292 (4)	C19—C28	1.408 (5)
O5—C8	1.303 (4)	C19—C20	1.432 (5)
O6—C8	1.215 (5)	C20—C21	1.341 (6)
O7—C14	1.213 (4)	C20—H20	0.9500
O8—C14	1.301 (4)	C21—C22	1.424 (6)
O9—H9B	0.9499	C21—H21	0.9500
O9—H9A	0.9497	C22—C27	1.396 (5)
O10—H10B	0.9500	C22—C23	1.409 (5)
O10—H10A	0.9502	C23—C24	1.351 (6)
C1—C2	1.514 (5)	C23—H23	0.9500
C2—C3	1.375 (5)	C24—C25	1.418 (6)
C3—C4	1.381 (5)	C24—H24	0.9500
C3—H3	0.9500	C25—C26	1.494 (6)
C4—C5	1.396 (5)	C26—H26C	0.9800
C4—H4	0.9500	C26—H26B	0.9800
C5—C6	1.361 (5)	C26—H26A	0.9800
C5—H5	0.9500	C27—C28	1.426 (5)
C6—C7	1.520 (5)		

O5—Fe1—O4	94.88 (11)	C12—C11—C10	121.1 (4)
O5—Fe1—O1	91.61 (11)	C12—C11—H11	119.4
O4—Fe1—O1	151.51 (10)	C10—C11—H11	119.4
O5—Fe1—O8	151.48 (11)	C11—C12—C13	118.0 (4)
O4—Fe1—O8	91.63 (11)	C11—C12—H12	121.0
O1—Fe1—O8	95.78 (12)	C13—C12—H12	121.0
O5—Fe1—N2	76.47 (12)	N2—C13—C12	120.2 (4)
O4—Fe1—N2	112.29 (11)	N2—C13—C14	111.3 (3)
O1—Fe1—N2	96.20 (11)	C12—C13—C14	128.5 (4)
O8—Fe1—N2	75.37 (12)	O7—C14—O8	125.8 (4)
O5—Fe1—N1	109.44 (11)	O7—C14—C13	121.3 (4)
O4—Fe1—N1	75.98 (11)	O8—C14—C13	112.9 (3)
O1—Fe1—N1	75.70 (11)	C16—C15—H15C	109.5
O8—Fe1—N1	99.08 (11)	C16—C15—H15B	109.5
N2—Fe1—N1	169.85 (12)	H15C—C15—H15B	109.5
C6—N1—C2	121.6 (3)	C16—C15—H15A	109.5
C6—N1—Fe1	118.9 (3)	H15C—C15—H15A	109.5
C2—N1—Fe1	119.4 (3)	H15B—C15—H15A	109.5
C9—N2—C13	121.9 (3)	N3—C16—C17	118.5 (4)
C9—N2—Fe1	118.6 (3)	N3—C16—C15	118.6 (4)

C13—N2—Fe1	119.4 (3)	C17—C16—C15	123.0 (4)
C16—N3—C28	123.7 (4)	C18—C17—C16	119.8 (4)
C16—N3—H3A	118.6	C18—C17—H17	120.1
C28—N3—H3A	117.7	C16—C17—H17	120.1
C25—N4—C27	117.5 (3)	C17—C18—C19	121.7 (4)
C1—O1—Fe1	120.4 (3)	C17—C18—H18	119.1
C7—O4—Fe1	121.3 (3)	C19—C18—H18	119.1
C8—O5—Fe1	120.6 (3)	C18—C19—C28	117.3 (4)
C14—O8—Fe1	120.9 (3)	C18—C19—C20	124.7 (4)
H9B—O9—H9A	97.1	C28—C19—C20	118.0 (4)
H10B—O10—H10A	105.9	C21—C20—C19	121.6 (4)
O2—C1—O1	125.9 (4)	C21—C20—H20	119.2
O2—C1—C2	120.4 (4)	C19—C20—H20	119.2
O1—C1—C2	113.7 (3)	C20—C21—C22	120.5 (4)
N1—C2—C3	121.3 (4)	C20—C21—H21	119.7
N1—C2—C1	110.7 (3)	C22—C21—H21	119.7
C3—C2—C1	127.9 (4)	C27—C22—C23	116.5 (4)
C2—C3—C4	117.8 (4)	C27—C22—C21	120.5 (4)
C2—C3—H3	121.1	C23—C22—C21	123.0 (4)
C4—C3—H3	121.1	C24—C23—C22	119.8 (4)
C3—C4—C5	119.6 (4)	C24—C23—H23	120.1
C3—C4—H4	120.2	C22—C23—H23	120.1
C5—C4—H4	120.2	C23—C24—C25	119.9 (4)
C6—C5—C4	119.3 (4)	C23—C24—H24	120.0
C6—C5—H5	120.4	C25—C24—H24	120.0
C4—C5—H5	120.4	N4—C25—C24	122.0 (4)
N1—C6—C5	120.4 (4)	N4—C25—C26	116.5 (4)
N1—C6—C7	110.9 (3)	C24—C25—C26	121.5 (4)
C5—C6—C7	128.7 (4)	C25—C26—H26C	109.5
O3—C7—O4	126.9 (4)	C25—C26—H26B	109.5
O3—C7—C6	120.2 (4)	H26C—C26—H26B	109.5
O4—C7—C6	112.8 (4)	C25—C26—H26A	109.5
O6—C8—O5	126.0 (4)	H26C—C26—H26A	109.5
O6—C8—C9	121.0 (4)	H26B—C26—H26A	109.5
O5—C8—C9	113.0 (4)	N4—C27—C22	124.3 (4)
N2—C9—C10	121.1 (4)	N4—C27—C28	117.3 (4)
N2—C9—C8	111.1 (3)	C22—C27—C28	118.4 (4)
C10—C9—C8	127.8 (4)	N3—C28—C19	119.0 (4)
C9—C10—C11	117.6 (4)	N3—C28—C27	119.9 (4)
C9—C10—H10	121.2	C19—C28—C27	121.0 (4)
C11—C10—H10	121.2		

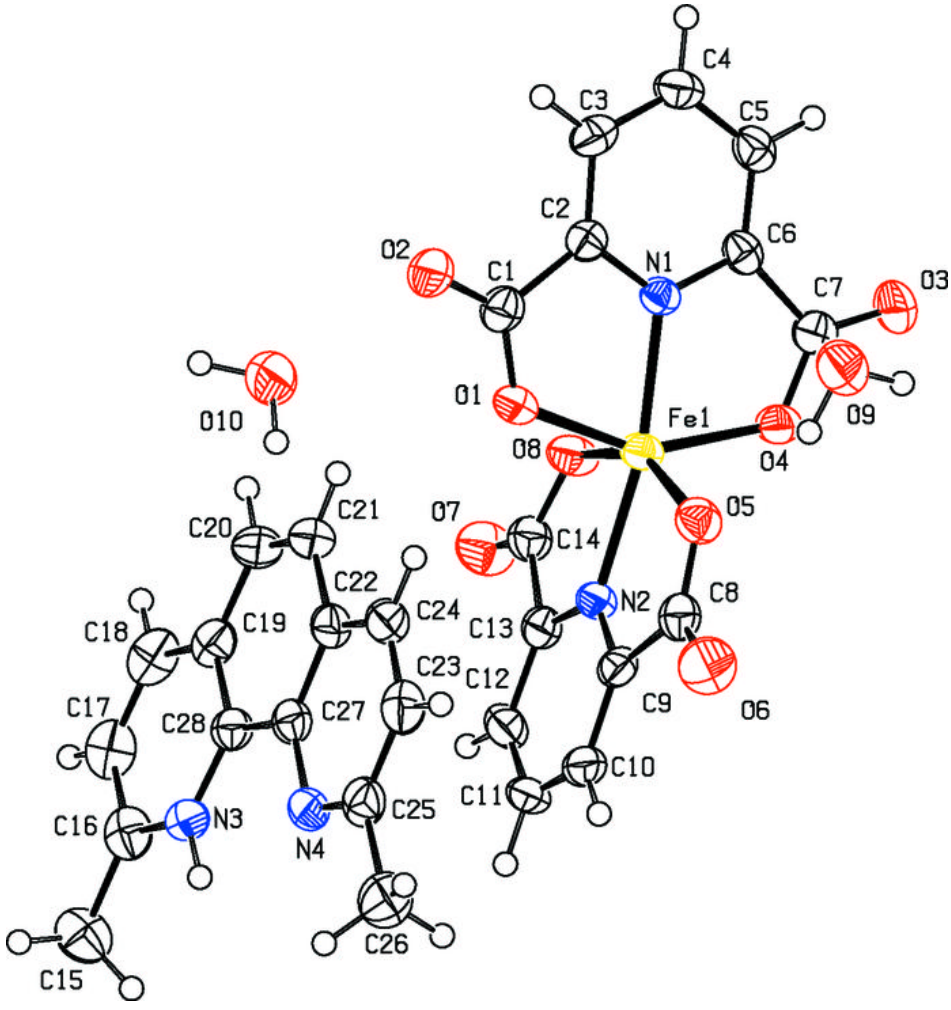
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9B···O10^{i}	0.95	2.01	2.907 (5)	157
O9—H9A···O5	0.95	1.99	2.866 (4)	153
O10—H10B···O9^{ii}	0.95	2.33	2.907 (4)	119

O10—H10A···O7^{iii}	0.95	2.11	2.964 (4)	150
N3—H3A···O8^{iv}	0.95	2.00	2.832 (4)	145
C3—H3···O7^{v}	0.95	2.45	3.304 (5)	150
C12—H12···O2^{vi}	0.95	2.39	3.263 (5)	152
C17—H17···O9^{vi}	0.95	2.41	3.357 (5)	175

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) *x*+1, *y*, *z*; (iv) *x*+1/2, −*y*+3/2, *z*+1/2; (v) *x*+1/2, −*y*+3/2, *z*−1/2; (vi) *x*−1/2, −*y*+3/2, *z*+1/2.

Fig. 1


C4
C3
C5
C2
O2
C1
N1
C6
C7
O3
O1
Fe1
O9
O10
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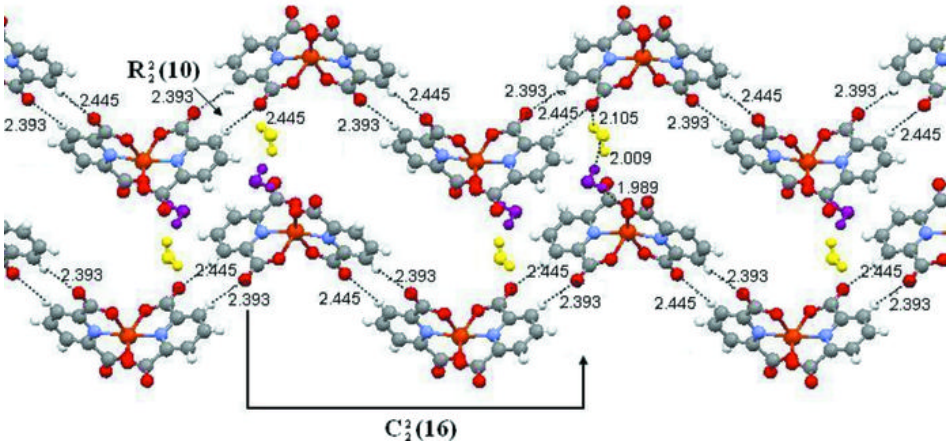
O4
C21
C20
O7
C14
O5
C22
N2
C8
C18
C19
C24
C13
C23
C12
C9
O6
C17
C28
C27
C10
C11
C16
N3
N4
C25
C26
C15

Fig. 2


$R_2^2(10)$
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2.393
2.445
2.393
2.445
2.393
2.445
2.393
2.105
2.009
1.989
2.393
2.445
2.393
2.445
2.393
2.445
2.393
2.445
2.393
2.445
2.393
$C_2^2(16)$

Fig. 3