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Piperazinediium bis[bis(pyridine-2,6-dicarboxylato)ferrate(III)] monohydrate

Hossein Aghabozorg,[a]* Andya Nemati,[a] Zohreh Derikvand[a] and Mohammad Ghadermazi[b]

[a]Faculty of Chemistry, Teacher Training University, 49 Mofateh Avenue 15614, Tehran, Iran, and [b]Department of Chemistry, University of Kurdistan, Sanandaj, Iran
Correspondence e-mail: haghabozorg@yahoo.com

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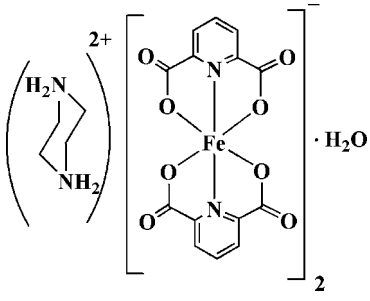
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.081; data-to-parameter ratio = 14.2.

The asymmetric unit of the title compound, $(C_4H_{12}N_2)$-$[Fe(C_7H_3NO_4)_2]_2\cdot H_2O$ or $(pipzH_2)^{2+}\cdot 2[Fe(pydc)_2]^{-}\cdot H_2O$ (pipz is piperazine and $pydcH_2$ is pyridine-2,6-dicarboxylic acid), contains one dication, two anions and one uncoordinated water molecule. In the anions, each Fe^{III} ion is hexacoordinated by four O [Fe—O = 2.005 (2)–2.044 (2) Å] and two N [Fe—N = 2.050 (2)–2.075 (2) Å] atoms in a distorted octahedral geometry. An extensive three-dimensional network formed by classical O—H···O and N—H···O and weak C—H···O intermolecular hydrogen bonds stabilizes the crystal packing, which also exhibits π–π [centroid–centroid distances 3.500 (2)–3.533 (2) Å] and C—H···π interactions.

Related literature

For related crystal structures, see: Aghabozorg, Attar Gharamaleki *et al.* (2007*a*,*b*); Aghabozorg, Motyeian *et al.* (2007); Aghabozorg, Sadrkhanlou *et al.* (2007); Sheshmani *et al.* (2006).



Experimental

Crystal data

$(C_4H_{12}N_2)\cdot[Fe(C_7H_3NO_4)_2]_2\cdot H_2O$
M_r = 878.29
Monoclinic, $P2_1/n$
a = 7.016 (3) Å
b = 24.855 (9) Å
c = 19.422 (7) Å
β = 98.697 (14)°
V = 3348 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 100 (2) K
0.23 × 0.15 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.795, T_{max} = 0.878
34715 measured reflections
7296 independent reflections
5113 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.081
S = 1.00
7296 reflections
514 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

*Cg*4 is the centroid of the N1/C1–C5 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···O8	0.90	1.94	2.836 (4)	175
N5—H5B···O4^{i}	0.90	1.88	2.742 (4)	161
N6—H6A···O11	0.90	1.94	2.816 (4)	165
N6—H6B···O14^{ii}	0.90	1.84	2.738 (4)	174
O1W—H1W···O2	0.85	1.95	2.805 (4)	176
O1W—H2W···O7^{iii}	0.87	2.01	2.837 (4)	160
C4—H4A···O10^{iv}	0.93	2.31	3.221 (4)	167
C9—H9A···O6^{v}	0.93	2.28	3.103 (4)	148
C11—H11A···O15^{vi}	0.93	2.39	3.126 (4)	136
C16—H16A···O1^{vii}	0.93	2.52	3.324 (4)	144
C17—H17A···O3^{viii}	0.93	2.51	3.237 (4)	135
C18—H18A···O12^{ix}	0.93	2.45	3.234 (4)	142
C25—H25A···O16^{iv}	0.93	2.33	3.223 (4)	162
C29—H29A···O10^{x}	0.97	2.38	3.171 (4)	138
C30—H30A···O1W	0.97	2.27	3.221 (4)	167
C31—H31B···O6^{xi}	0.97	2.45	3.135 (4)	127
C32—H32A···O1W^{ii}	0.97	2.59	3.495 (4)	155
C32—H32B···O5^{xi}	0.97	2.54	3.340 (4)	140
C23—H23A···*Cg*4^{iii}	0.93	2.81	3.591 (4)	142

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2339).

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supplementary materials

Acta Cryst. (2007). E**63**, m2921 [**doi:10.1107/S1600536807055468**]

Piperazinediium bis[bis(pyridine-2,6-dicarboxylato)ferrate(III)] monohydrate

H. Aghabozorg, A. Nemati, Z. Derikvand and M. Ghadermazi

Comment

Recent interest of our research group has focused on self-assembling synthesis and characterization of novel metal complexes of proton transfer compounds (Aghabozorg, Sadrkhanlou *et al.*, 2007; Aghabozorg, Motyeian *et al.*, 2007; Aghabozorg, Attar Gharamaleki *et al.*, 2007*a*,b). The pyridine-2,6-dicarboxylate ion is an effective tridentate chelating ligand forming stable complexes with most metal ions (Sheshmani *et al.*, 2006). This compound has not been crystallized until now but its metal-organic derivatives can be obtained as suitable crystals. We have recently reported the crystal structures of new compounds synthesized using this ligand and piperazinediium as counter-ion. In this report, the crystal structure of the title iron(III) derivative, (I), is described.

The $Fe1^{III}$ and $Fe2^{III}$ ions are located at the centers of a distorted octahedrons (Fig.1). The angles N1—Fe1—N2 [169.31 (10)°], O1—Fe1—O3 [151.57 (9)°], O5—Fe1—O7 [151.57 (8)°], N3—Fe2—N4 [170.52 (10)°], O9—Fe2—O11 [151.29 (8)°] and O13—Fe2—O15 [151.16 (8)°] indicate some difference in $Fe1^{III}$ and $Fe2^{III}$ coordination geometries.

The torsion angles C7—O3—Fe1—O5 [86.8 (2)°] and C6— O1—Fe1—O5 [−91.3 (2)°] indicate that two dianionic $pydc^{2-}$ units connecting to $Fe1^{III}$ ion,are almost perpendicular to each other. The same is valid for Fe2 center, proved by torsion angles C27— O13—Fe2—O9 [92.4 (2)°] and C28— O15—Fe2—O9 [−90.1 (2)°]

In this work we use Fe^{2+} ions as starting material. Most probably, during the synthesis, Fe^{2+} ions oxidize into Fe^{3+} ions and in our crystalline product we obtain Fe^{III} complexes.

There are π-π stacking interactions between the anions, proved by short distances $Cg1\cdots Cg2^{i}$, $Cg1\cdots Cg2^{ii}$ and $Cg3\cdots Cg3^{iii}$ of 3.500 (2), 3.533 (2) and 3.724 (2) Å, respectively [*Cg*1, *Cg*2 and *Cg*3 are centroids of N2/C8—C12, N3/C15—C19 and N4/C22—C26 rings, respectively. Symmetry codes: (i) 1/2 − *x*, −1/2 + *y*, 1/2-*z* ; (ii) 3/2 − *x*, −1/2 + *y*, 1/2 − *z*; (iii) −*x*, 1 − *y*, −*z*]. Also C—H···π interactions exist in the crystal, with $C23\cdots Cg4^{iv}$ distance of 3.591 (4) Å (Fig. 2) [symmetry code: (iv) −1 + *x*, *y*, *z*]. The extensive O—H···O, N—H···O and C—H···O hydrogen bonds (Table 1) between $[Fe1(pydc)_2]^-$, $[Fe2(pydc)_2]^-$, $(pipzH_2)^{2+}$ and uncoordinated water molecules play an important role in stabilization of the crystal packing (Fig. 3).

Experimental

The proton transfer compound $(pipzH_2)(pydcH)_2\cdot 3H_2O$, was prepared by the reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) with piperazine (pipz), (Sheshmani *et al.*, 2006). The reaction between $FeSO_4\cdot 7H_2O$ (139 mg, 0.5 mmol) in water (25 ml) and the proton transfer compound $(pipzH_2)(pydcH)_2\cdot 3H_2O$ (253 mg, 1.0 mmol) in water (25 ml), in a 1:2 molar ratio was carried by slow evaporation of the solvent at room temperature.

Refinement

The C– and N-bound H atoms were geometrically positioned (C—H 0.93–0.97 Å, N—H 0.90 Å). Hydrogen atoms of water molecule were found in difference Fourier map and placed in idealized positions with O—H = 0.85, 0.87 Å. All hydrogen atoms were refined in riding model, with U_{iso}(H) = 1.2 U_{eq} of the parent atom.

Figures

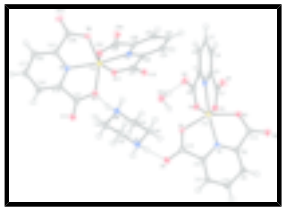

Fig. 1. **Fig. 1.** The content of asymmetric unit of compound (I) showing the atomic numbering and displacement ellipsoids at the 50% proability level. Hydrogen bonds are shown as dashed lines.

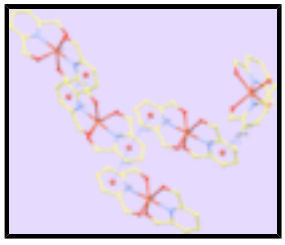

Fig. 2. **Fig. 2.** Intermolecular π-π and C—H···π interactions (dashed lines) between anionic fragments in (I).

Fig. 3. **Fig.3** A portion of the crystal packing viewed approximately down the *a* axis. Hydrogen bonds are shown as dashed lines.

Piperazinediium bis[bis(pyridine-2,6-dicarboxylato)ferrate(III)] monohydrate

Crystal data

$(C_4H_{12}N_2)\cdot[Fe(C_7H_3NO_4)_2]_2\cdot H_2O$	F_{000} = 1792
M_r = 878.29	D_x = 1.743 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.016 (3) Å	Cell parameters from 3260 reflections
b = 24.855 (9) Å	θ = 3–25°
c = 19.422 (7) Å	μ = 0.96 mm^{-1}
β = 98.697 (14)°	T = 100 (2) K
V = 3348 (2) Å^3	Prism, light yellow
Z = 4	0.23 × 0.15 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	7296 independent reflections
Radiation source: fine-focus sealed tube	5113 reflections with $I > 2u(I)$
Monochromator: graphite	$R_{int} = 0.090$
$T = 100(2)$ K	$\theta_{max} = 27.0°$
phi and ω scans	$\theta_{min} = 2.0°$
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -8\rightarrow8$
$T_{min} = 0.795$, $T_{max} = 0.878$	$k = -31\rightarrow31$
34715 measured reflections	$l = -24\rightarrow24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 5.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
7296 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
514 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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	0.71620 (6)	0.207066 (17)	0.04276 (2)	0.01291 (11)
O1	0.4764 (3)	0.24328 (8)	0.06569 (11)	0.0166 (5)
O2	0.2727 (3)	0.31326 (9)	0.04273 (12)	0.0211 (5)
O3	0.9642 (3)	0.20780 (8)	0.00102 (11)	0.0165 (5)
O4	1.1158 (3)	0.24126 (9)	−0.08327 (11)	0.0207 (5)
O5	0.5842 (3)	0.15623 (8)	−0.02932 (11)	0.0163 (5)

O6	0.5183 (3)	0.06986 (8)	−0.05937 (11)	0.0174 (5)
O7	0.8526 (3)	0.22327 (8)	0.14032 (10)	0.0156 (5)
O8	0.9823 (3)	0.19068 (8)	0.24467 (11)	0.0175 (5)
N1	0.6895 (4)	0.27400 (9)	−0.01967 (13)	0.0121 (5)
N2	0.7583 (3)	0.13279 (10)	0.08960 (12)	0.0116 (5)
C1	0.5311 (4)	0.30378 (12)	−0.02266 (15)	0.0137 (7)
C2	0.4961 (5)	0.34517 (12)	−0.07039 (16)	0.0171 (7)
H2A	0.3861	0.3664	−0.0727	0.021*
C3	0.6304 (5)	0.35402 (12)	−0.11464 (16)	0.0176 (7)
H3A	0.6095	0.3814	−0.1476	0.021*
C4	0.7966 (5)	0.32254 (12)	−0.11064 (16)	0.0174 (7)
H4A	0.8875	0.3287	−0.1400	0.021*
C5	0.8212 (4)	0.28188 (12)	−0.06154 (15)	0.0133 (7)
C6	0.4107 (4)	0.28637 (12)	0.03254 (15)	0.0141 (7)
C7	0.9836 (4)	0.24122 (12)	−0.04780 (15)	0.0142 (7)
C8	0.6869 (4)	0.08948 (12)	0.05390 (15)	0.0125 (6)
C9	0.6972 (4)	0.03904 (12)	0.08467 (16)	0.0138 (7)
H9A	0.6493	0.0087	0.0600	0.017*
C10	0.7826 (4)	0.03575 (12)	0.15446 (16)	0.0146 (7)
H10A	0.7899	0.0026	0.1769	0.018*
C11	0.8566 (4)	0.08114 (12)	0.19087 (16)	0.0135 (7)
H11A	0.9132	0.0789	0.2373	0.016*
C12	0.8435 (4)	0.12969 (12)	0.15588 (15)	0.0123 (6)
C13	0.5878 (4)	0.10475 (12)	−0.01869 (15)	0.0129 (7)
C14	0.9016 (4)	0.18461 (12)	0.18457 (16)	0.0139 (7)
Fe2	0.13045 (6)	0.498478 (18)	0.22775 (2)	0.01192 (10)
O9	0.0081 (3)	0.57045 (8)	0.19928 (10)	0.0158 (5)
O10	−0.0516 (3)	0.65490 (8)	0.23228 (11)	0.0192 (5)
O11	0.2693 (3)	0.44742 (8)	0.30124 (10)	0.0139 (5)
O12	0.4383 (3)	0.43939 (9)	0.40847 (11)	0.0174 (5)
O13	−0.1175 (3)	0.45562 (8)	0.22040 (10)	0.0155 (5)
O14	−0.3321 (3)	0.40362 (8)	0.15340 (11)	0.0171 (5)
O15	0.3776 (3)	0.51753 (8)	0.19324 (10)	0.0161 (5)
O16	0.5341 (3)	0.52268 (8)	0.10081 (11)	0.0180 (5)
N3	0.1764 (3)	0.54382 (10)	0.31847 (12)	0.0110 (5)
N4	0.1015 (4)	0.46452 (10)	0.13012 (13)	0.0126 (5)
C15	0.1258 (4)	0.59589 (12)	0.31464 (16)	0.0132 (7)
C16	0.1758 (4)	0.62933 (12)	0.37140 (16)	0.0152 (7)
H16A	0.1431	0.6656	0.3689	0.018*
C17	0.2763 (4)	0.60755 (13)	0.43247 (16)	0.0153 (7)
H17A	0.3119	0.6294	0.4711	0.018*
C18	0.3234 (4)	0.55302 (12)	0.43571 (15)	0.0137 (7)
H18A	0.3860	0.5377	0.4767	0.016*
C19	0.2742 (4)	0.52220 (12)	0.37614 (15)	0.0123 (6)
C20	0.0167 (4)	0.60987 (12)	0.24339 (16)	0.0150 (7)
C21	0.3333 (4)	0.46497 (12)	0.36450 (15)	0.0124 (6)
C22	−0.0591 (4)	0.43742 (12)	0.10654 (15)	0.0124 (6)
C23	−0.0907 (4)	0.41764 (12)	0.03954 (16)	0.0157 (7)
H23A	−0.2026	0.3987	0.0229	0.019*

C24	0.0505 (5)	0.42688 (12)	−0.00249 (16)	0.0173 (7)
H24A	0.0324	0.4142	−0.0481	0.021*
C25	0.2179 (5)	0.45485 (12)	0.02302 (15)	0.0145 (7)
H25A	0.3134	0.4607	−0.0045	0.017*
C26	0.2377 (4)	0.47350 (12)	0.09018 (16)	0.0129 (6)
C27	−0.1845 (4)	0.43116 (12)	0.16316 (16)	0.0140 (7)
C28	0.4009 (4)	0.50685 (12)	0.12910 (15)	0.0129 (6)
N5	0.7543 (4)	0.27251 (11)	0.29327 (13)	0.0203 (6)
H5A	0.8324	0.2478	0.2784	0.024*
H5B	0.7175	0.2602	0.3328	0.024*
N6	0.5561 (4)	0.37357 (10)	0.27689 (13)	0.0166 (6)
H6A	0.4776	0.3982	0.2918	0.020*
H6B	0.5913	0.3858	0.2370	0.020*
C29	0.5805 (5)	0.28004 (13)	0.23931 (17)	0.0209 (8)
H29A	0.5115	0.2462	0.2314	0.025*
H29B	0.6200	0.2912	0.1958	0.025*
C30	0.4504 (5)	0.32196 (12)	0.26320 (17)	0.0185 (7)
H30A	0.3391	0.3273	0.2277	0.022*
H30B	0.4052	0.3098	0.3054	0.022*
C31	0.7309 (5)	0.36691 (13)	0.33023 (16)	0.0189 (7)
H31A	0.6925	0.3568	0.3744	0.023*
H31B	0.7997	0.4008	0.3367	0.023*
C32	0.8625 (5)	0.32418 (13)	0.30800 (17)	0.0209 (7)
H32A	0.9122	0.3360	0.2665	0.025*
H32B	0.9710	0.3186	0.3446	0.025*
O1W	0.0582 (3)	0.32196 (9)	0.15291 (11)	0.0226 (5)
H1W	0.1188	0.3197	0.1181	0.027*
H2W	0.0181	0.2892	0.1568	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0157 (2)	0.0105 (2)	0.0122 (2)	0.00008 (19)	0.00130 (18)	0.00209 (18)
O1	0.0188 (12)	0.0156 (12)	0.0168 (12)	0.0003 (10)	0.0070 (9)	0.0033 (9)
O2	0.0193 (13)	0.0191 (12)	0.0262 (13)	0.0045 (10)	0.0079 (10)	−0.0017 (10)
O3	0.0163 (12)	0.0166 (11)	0.0167 (11)	0.0039 (10)	0.0033 (9)	0.0028 (10)
O4	0.0174 (12)	0.0284 (13)	0.0176 (12)	0.0019 (10)	0.0073 (10)	−0.0019 (10)
O5	0.0185 (12)	0.0131 (11)	0.0160 (11)	0.0004 (9)	−0.0018 (9)	0.0015 (9)
O6	0.0177 (12)	0.0165 (12)	0.0180 (12)	−0.0033 (10)	0.0023 (9)	−0.0029 (10)
O7	0.0211 (12)	0.0109 (11)	0.0142 (11)	0.0005 (9)	0.0010 (9)	0.0014 (9)
O8	0.0178 (12)	0.0189 (12)	0.0148 (12)	0.0027 (10)	−0.0004 (9)	−0.0017 (9)
N1	0.0132 (13)	0.0103 (13)	0.0125 (13)	−0.0005 (11)	0.0005 (10)	−0.0016 (11)
N2	0.0108 (13)	0.0119 (13)	0.0129 (13)	0.0017 (10)	0.0042 (10)	0.0007 (11)
C1	0.0137 (16)	0.0122 (16)	0.0139 (16)	−0.0014 (13)	−0.0016 (13)	−0.0035 (12)
C2	0.0228 (18)	0.0126 (16)	0.0146 (16)	0.0010 (14)	−0.0017 (14)	−0.0013 (13)
C3	0.0299 (19)	0.0080 (15)	0.0137 (16)	−0.0013 (14)	0.0000 (14)	−0.0001 (13)
C4	0.0249 (18)	0.0159 (16)	0.0123 (16)	−0.0038 (14)	0.0061 (14)	−0.0020 (13)
C5	0.0140 (16)	0.0146 (16)	0.0107 (15)	−0.0030 (13)	0.0000 (12)	−0.0033 (12)

C6	0.0143 (16)	0.0154 (16)	0.0125 (16)	−0.0007 (14)	0.0014 (12)	−0.0010 (13)
C7	0.0160 (17)	0.0146 (16)	0.0110 (15)	−0.0023 (13)	−0.0009 (13)	−0.0042 (13)
C8	0.0090 (15)	0.0135 (16)	0.0161 (16)	0.0024 (13)	0.0051 (12)	−0.0005 (13)
C9	0.0120 (16)	0.0097 (15)	0.0209 (17)	0.0007 (13)	0.0065 (13)	−0.0010 (13)
C10	0.0138 (16)	0.0108 (15)	0.0205 (17)	0.0036 (13)	0.0064 (13)	0.0050 (13)
C11	0.0135 (16)	0.0150 (16)	0.0130 (16)	0.0059 (13)	0.0052 (13)	0.0029 (13)
C12	0.0087 (15)	0.0173 (16)	0.0116 (15)	0.0031 (13)	0.0035 (12)	0.0005 (13)
C13	0.0095 (15)	0.0173 (17)	0.0130 (16)	−0.0001 (13)	0.0055 (12)	−0.0024 (13)
C14	0.0122 (16)	0.0155 (16)	0.0150 (17)	0.0027 (13)	0.0055 (13)	0.0001 (13)
Fe2	0.0134 (2)	0.0123 (2)	0.0103 (2)	−0.00072 (19)	0.00259 (17)	−0.00144 (18)
O9	0.0195 (12)	0.0147 (11)	0.0124 (11)	−0.0005 (10)	0.0002 (9)	0.0002 (9)
O10	0.0218 (13)	0.0143 (12)	0.0228 (12)	0.0033 (10)	0.0082 (10)	0.0048 (10)
O11	0.0163 (12)	0.0135 (11)	0.0123 (11)	0.0023 (9)	0.0034 (9)	−0.0015 (9)
O12	0.0169 (12)	0.0194 (12)	0.0152 (12)	0.0041 (10)	0.0000 (9)	0.0025 (10)
O13	0.0166 (12)	0.0159 (12)	0.0144 (11)	−0.0004 (9)	0.0041 (9)	−0.0024 (9)
O14	0.0158 (12)	0.0179 (12)	0.0172 (12)	−0.0049 (10)	0.0014 (9)	−0.0005 (9)
O15	0.0154 (12)	0.0208 (12)	0.0130 (11)	−0.0039 (9)	0.0046 (9)	−0.0034 (9)
O16	0.0170 (12)	0.0188 (12)	0.0193 (12)	−0.0035 (10)	0.0065 (10)	−0.0004 (10)
N3	0.0088 (13)	0.0121 (13)	0.0131 (13)	−0.0005 (10)	0.0046 (10)	−0.0021 (10)
N4	0.0148 (14)	0.0109 (13)	0.0128 (13)	0.0019 (11)	0.0044 (11)	0.0005 (11)
C15	0.0122 (16)	0.0134 (16)	0.0160 (16)	−0.0003 (13)	0.0086 (13)	0.0004 (13)
C16	0.0138 (16)	0.0139 (16)	0.0203 (17)	−0.0014 (13)	0.0109 (13)	−0.0030 (13)
C17	0.0105 (16)	0.0205 (17)	0.0159 (16)	−0.0043 (13)	0.0059 (13)	−0.0085 (13)
C18	0.0103 (16)	0.0205 (17)	0.0109 (15)	−0.0020 (13)	0.0038 (12)	−0.0003 (13)
C19	0.0097 (15)	0.0157 (16)	0.0125 (15)	−0.0010 (13)	0.0047 (12)	0.0013 (13)
C20	0.0119 (16)	0.0160 (17)	0.0189 (17)	−0.0028 (13)	0.0078 (13)	0.0027 (14)
C21	0.0108 (15)	0.0150 (16)	0.0127 (16)	−0.0023 (13)	0.0056 (12)	−0.0005 (13)
C22	0.0147 (16)	0.0089 (15)	0.0127 (15)	0.0001 (13)	−0.0006 (12)	0.0009 (12)
C23	0.0152 (17)	0.0142 (16)	0.0166 (16)	−0.0008 (13)	−0.0007 (13)	−0.0013 (13)
C24	0.0289 (19)	0.0122 (16)	0.0104 (15)	0.0011 (14)	0.0022 (14)	−0.0021 (13)
C25	0.0205 (17)	0.0121 (16)	0.0119 (16)	0.0016 (13)	0.0055 (13)	0.0007 (13)
C26	0.0155 (16)	0.0076 (15)	0.0159 (16)	0.0007 (13)	0.0038 (13)	0.0019 (12)
C27	0.0154 (17)	0.0113 (16)	0.0146 (16)	0.0012 (13)	0.0004 (13)	0.0030 (13)
C28	0.0138 (16)	0.0112 (16)	0.0144 (15)	0.0041 (13)	0.0042 (12)	0.0020 (13)
N5	0.0276 (16)	0.0215 (15)	0.0125 (14)	0.0096 (13)	0.0055 (12)	0.0026 (12)
N6	0.0182 (15)	0.0155 (14)	0.0171 (14)	0.0019 (12)	0.0058 (11)	−0.0023 (11)
C29	0.027 (2)	0.0171 (18)	0.0182 (17)	−0.0006 (14)	0.0004 (15)	−0.0008 (14)
C30	0.0163 (17)	0.0156 (17)	0.0238 (18)	−0.0012 (14)	0.0037 (14)	0.0015 (14)
C31	0.0204 (18)	0.0203 (18)	0.0158 (17)	−0.0035 (14)	0.0018 (14)	−0.0036 (14)
C32	0.0147 (17)	0.030 (2)	0.0180 (17)	0.0030 (15)	0.0021 (14)	0.0005 (15)
O1W	0.0269 (14)	0.0192 (12)	0.0228 (13)	−0.0035 (10)	0.0077 (10)	−0.0009 (10)

Geometric parameters (Å, °)

Fe1—O5	2.005 (2)	O13—C27	1.292 (3)
Fe1—O1	2.017 (2)	O14—C27	1.232 (4)
Fe1—O3	2.028 (2)	O15—C28	1.308 (3)
Fe1—O7	2.030 (2)	O16—C28	1.219 (3)
Fe1—N1	2.050 (2)	N3—C19	1.335 (4)

Fe1—N2	2.060 (3)	N3—C15	1.341 (4)
O1—C6	1.297 (4)	N4—C22	1.333 (4)
O2—C6	1.217 (4)	N4—C26	1.338 (4)
O3—C7	1.283 (4)	C15—C16	1.383 (4)
O4—C7	1.236 (3)	C15—C20	1.517 (4)
O5—C13	1.296 (4)	C16—C17	1.394 (4)
O6—C13	1.224 (3)	C16—H16A	0.9300
O7—C14	1.300 (3)	C17—C18	1.394 (4)
O8—C14	1.227 (4)	C17—H17A	0.9300
N1—C1	1.329 (4)	C18—C19	1.387 (4)
N1—C5	1.335 (4)	C18—H18A	0.9300
N2—C8	1.336 (4)	C19—C21	1.508 (4)
N2—C12	1.337 (4)	C22—C23	1.377 (4)
C1—C2	1.382 (4)	C22—C27	1.517 (4)
C1—C6	1.524 (4)	C23—C24	1.395 (4)
C2—C3	1.385 (4)	C23—H23A	0.9300
C2—H2A	0.9300	C24—C25	1.390 (4)
C3—C4	1.397 (4)	C24—H24A	0.9300
C3—H3A	0.9300	C25—C26	1.371 (4)
C4—C5	1.382 (4)	C25—H25A	0.9300
C4—H4A	0.9300	C26—C28	1.519 (4)
C5—C7	1.516 (4)	N5—C29	1.494 (4)
C8—C9	1.386 (4)	N5—C32	1.497 (4)
C8—C13	1.523 (4)	N5—H5A	0.9000
C9—C10	1.399 (4)	N5—H5B	0.9000
C9—H9A	0.9300	N6—C30	1.485 (4)
C10—C11	1.390 (4)	N6—C31	1.490 (4)
C10—H10A	0.9300	N6—H6A	0.9000
C11—C12	1.381 (4)	N6—H6B	0.9000
C11—H11A	0.9300	C29—C30	1.504 (4)
C12—C14	1.507 (4)	C29—H29A	0.9700
Fe2—O15	2.008 (2)	C29—H29B	0.9700
Fe2—O9	2.025 (2)	C30—H30A	0.9700
Fe2—O13	2.026 (2)	C30—H30B	0.9700
Fe2—O11	2.044 (2)	C31—C32	1.512 (4)
Fe2—N4	2.057 (3)	C31—H31A	0.9700
Fe2—N3	2.075 (2)	C31—H31B	0.9700
O9—C20	1.297 (4)	C32—H32A	0.9700
O10—C20	1.224 (4)	C32—H32B	0.9700
O11—C21	1.317 (3)	O1W—H1W	0.8540
O12—C21	1.219 (3)	O1W—H2W	0.8677
O5—Fe1—O1	97.06 (9)	C19—N3—C15	122.2 (3)
O5—Fe1—O3	93.44 (9)	C19—N3—Fe2	119.2 (2)
O1—Fe1—O3	151.57 (9)	C15—N3—Fe2	118.1 (2)
O5—Fe1—O7	151.57 (8)	C22—N4—C26	121.7 (3)
O1—Fe1—O7	89.81 (9)	C22—N4—Fe2	119.0 (2)
O3—Fe1—O7	93.41 (9)	C26—N4—Fe2	119.1 (2)
O5—Fe1—N1	96.14 (9)	N3—C15—C16	120.2 (3)
O1—Fe1—N1	76.33 (9)	N3—C15—C20	111.4 (3)

O3—Fe1—N1	76.32 (9)	C16—C15—C20	128.4 (3)
O7—Fe1—N1	112.28 (9)	C15—C16—C17	118.6 (3)
O5—Fe1—N2	76.34 (9)	C15—C16—H16A	120.7
O1—Fe1—N2	111.80 (9)	C17—C16—H16A	120.7
O3—Fe1—N2	96.32 (9)	C18—C17—C16	120.1 (3)
O7—Fe1—N2	75.50 (9)	C18—C17—H17A	119.9
N1—Fe1—N2	169.31 (10)	C16—C17—H17A	119.9
C6—O1—Fe1	120.28 (19)	C19—C18—C17	118.2 (3)
C7—O3—Fe1	119.63 (19)	C19—C18—H18A	120.9
C13—O5—Fe1	121.01 (19)	C17—C18—H18A	120.9
C14—O7—Fe1	120.71 (19)	N3—C19—C18	120.6 (3)
C1—N1—C5	122.9 (3)	N3—C19—C21	111.8 (3)
C1—N1—Fe1	118.6 (2)	C18—C19—C21	127.3 (3)
C5—N1—Fe1	118.0 (2)	O10—C20—O9	126.6 (3)
C8—N2—C12	122.1 (3)	O10—C20—C15	120.0 (3)
C8—N2—Fe1	118.4 (2)	O9—C20—C15	113.4 (3)
C12—N2—Fe1	119.4 (2)	O12—C21—O11	124.4 (3)
N1—C1—C2	120.4 (3)	O12—C21—C19	122.5 (3)
N1—C1—C6	111.1 (3)	O11—C21—C19	112.9 (3)
C2—C1—C6	128.5 (3)	N4—C22—C23	120.8 (3)
C1—C2—C3	117.8 (3)	N4—C22—C27	110.8 (3)
C1—C2—H2A	121.1	C23—C22—C27	128.3 (3)
C3—C2—H2A	121.1	C22—C23—C24	117.8 (3)
C2—C3—C4	121.1 (3)	C22—C23—H23A	121.1
C2—C3—H3A	119.4	C24—C23—H23A	121.1
C4—C3—H3A	119.4	C25—C24—C23	120.7 (3)
C5—C4—C3	117.6 (3)	C25—C24—H24A	119.7
C5—C4—H4A	121.2	C23—C24—H24A	119.7
C3—C4—H4A	121.2	C26—C25—C24	117.8 (3)
N1—C5—C4	120.1 (3)	C26—C25—H25A	121.1
N1—C5—C7	111.5 (3)	C24—C25—H25A	121.1
C4—C5—C7	128.4 (3)	N4—C26—C25	121.1 (3)
O2—C6—O1	127.1 (3)	N4—C26—C28	110.7 (3)
O2—C6—C1	119.8 (3)	C25—C26—C28	128.2 (3)
O1—C6—C1	113.0 (3)	O14—C27—O13	125.6 (3)
O4—C7—O3	125.8 (3)	O14—C27—C22	120.8 (3)
O4—C7—C5	120.6 (3)	O13—C27—C22	113.6 (3)
O3—C7—C5	113.6 (3)	O16—C28—O15	125.4 (3)
N2—C8—C9	120.9 (3)	O16—C28—C26	121.6 (3)
N2—C8—C13	111.3 (3)	O15—C28—C26	113.0 (2)
C9—C8—C13	127.7 (3)	C29—N5—C32	111.3 (2)
C8—C9—C10	117.2 (3)	C29—N5—H5A	109.4
C8—C9—H9A	121.4	C32—N5—H5A	109.4
C10—C9—H9A	121.4	C29—N5—H5B	109.4
C11—C10—C9	121.2 (3)	C32—N5—H5B	109.4
C11—C10—H10A	119.4	H5A—N5—H5B	108.0
C9—C10—H10A	119.4	C30—N6—C31	111.4 (2)
C12—C11—C10	117.8 (3)	C30—N6—H6A	109.4
C12—C11—H11A	121.1	C31—N6—H6A	109.4

C10—C11—H11A	121.1	C30—N6—H6B	109.4
N2—C12—C11	120.7 (3)	C31—N6—H6B	109.4
N2—C12—C14	111.1 (3)	H6A—N6—H6B	108.0
C11—C12—C14	128.0 (3)	N5—C29—C30	109.8 (3)
O6—C13—O5	126.9 (3)	N5—C29—H29A	109.7
O6—C13—C8	120.2 (3)	C30—C29—H29A	109.7
O5—C13—C8	112.9 (3)	N5—C29—H29B	109.7
O8—C14—O7	125.2 (3)	C30—C29—H29B	109.7
O8—C14—C12	121.5 (3)	H29A—C29—H29B	108.2
O7—C14—C12	113.3 (3)	N6—C30—C29	110.1 (3)
O15—Fe2—O9	93.01 (9)	N6—C30—H30A	109.6
O15—Fe2—O13	151.16 (8)	C29—C30—H30A	109.6
O9—Fe2—O13	96.96 (9)	N6—C30—H30B	109.6
O15—Fe2—O11	92.01 (9)	C29—C30—H30B	109.6
O9—Fe2—O11	151.29 (8)	H30A—C30—H30B	108.2
O13—Fe2—O11	92.08 (9)	N6—C31—C32	110.7 (3)
O15—Fe2—N4	76.05 (9)	N6—C31—H31A	109.5
O9—Fe2—N4	97.59 (9)	C32—C31—H31A	109.5
O13—Fe2—N4	75.84 (9)	N6—C31—H31B	109.5
O11—Fe2—N4	111.05 (9)	C32—C31—H31B	109.5
O15—Fe2—N3	97.14 (9)	H31A—C31—H31B	108.1
O9—Fe2—N3	75.94 (9)	N5—C32—C31	110.1 (3)
O13—Fe2—N3	111.51 (9)	N5—C32—H32A	109.6
O11—Fe2—N3	75.39 (9)	C31—C32—H32A	109.6
N4—Fe2—N3	170.52 (10)	N5—C32—H32B	109.6
C20—O9—Fe2	120.76 (19)	C31—C32—H32B	109.6
C21—O11—Fe2	120.34 (18)	H32A—C32—H32B	108.2
C27—O13—Fe2	120.33 (19)	H1W—O1W—H2W	102.4
C28—O15—Fe2	120.59 (19)		
O5—Fe1—O1—C6	−91.3 (2)	O13—Fe2—O9—C20	113.2 (2)
O3—Fe1—O1—C6	19.5 (3)	O11—Fe2—O9—C20	5.8 (3)
O7—Fe1—O1—C6	116.3 (2)	N4—Fe2—O9—C20	−170.2 (2)
N1—Fe1—O1—C6	3.3 (2)	N3—Fe2—O9—C20	2.7 (2)
N2—Fe1—O1—C6	−169.4 (2)	O15—Fe2—O11—C21	91.7 (2)
O5—Fe1—O3—C7	86.8 (2)	O9—Fe2—O11—C21	−8.3 (3)
O1—Fe1—O3—C7	−24.9 (3)	O13—Fe2—O11—C21	−116.8 (2)
O7—Fe1—O3—C7	−120.8 (2)	N4—Fe2—O11—C21	167.5 (2)
N1—Fe1—O3—C7	−8.7 (2)	N3—Fe2—O11—C21	−5.2 (2)
N2—Fe1—O3—C7	163.4 (2)	O15—Fe2—O13—C27	−17.0 (3)
O1—Fe1—O5—C13	−113.5 (2)	O9—Fe2—O13—C27	92.4 (2)
O3—Fe1—O5—C13	93.0 (2)	O11—Fe2—O13—C27	−114.9 (2)
O7—Fe1—O5—C13	−10.7 (3)	N4—Fe2—O13—C27	−3.7 (2)
N1—Fe1—O5—C13	169.6 (2)	N3—Fe2—O13—C27	170.0 (2)
N2—Fe1—O5—C13	−2.7 (2)	O9—Fe2—O15—C28	−90.1 (2)
O5—Fe1—O7—C14	8.1 (3)	O13—Fe2—O15—C28	20.2 (3)
O1—Fe1—O7—C14	112.7 (2)	O11—Fe2—O15—C28	118.2 (2)
O3—Fe1—O7—C14	−95.6 (2)	N4—Fe2—O15—C28	7.0 (2)
N1—Fe1—O7—C14	−172.2 (2)	N3—Fe2—O15—C28	−166.3 (2)
N2—Fe1—O7—C14	0.1 (2)	O15—Fe2—N3—C19	−86.9 (2)

O5—Fe1—N1—C1	88.3 (2)	O9—Fe2—N3—C19	−178.3 (2)
O1—Fe1—N1—C1	−7.5 (2)	O13—Fe2—N3—C19	89.7 (2)
O3—Fe1—N1—C1	−179.6 (2)	O11—Fe2—N3—C19	3.3 (2)
O7—Fe1—N1—C1	−91.5 (2)	O15—Fe2—N3—C15	85.4 (2)
N2—Fe1—N1—C1	133.1 (5)	O9—Fe2—N3—C15	−5.9 (2)
O5—Fe1—N1—C5	−83.9 (2)	O13—Fe2—N3—C15	−98.0 (2)
O1—Fe1—N1—C5	−179.7 (2)	O11—Fe2—N3—C15	175.6 (2)
O3—Fe1—N1—C5	8.2 (2)	O15—Fe2—N4—C22	179.6 (2)
O7—Fe1—N1—C5	96.3 (2)	O9—Fe2—N4—C22	−89.1 (2)
N2—Fe1—N1—C5	−39.1 (6)	O13—Fe2—N4—C22	6.2 (2)
O5—Fe1—N2—C8	0.4 (2)	O11—Fe2—N4—C22	92.9 (2)
O1—Fe1—N2—C8	92.6 (2)	O15—Fe2—N4—C26	−5.2 (2)
O3—Fe1—N2—C8	−91.6 (2)	O9—Fe2—N4—C26	86.1 (2)
O7—Fe1—N2—C8	176.5 (2)	O13—Fe2—N4—C26	−178.6 (2)
N1—Fe1—N2—C8	−45.7 (6)	O11—Fe2—N4—C26	−91.9 (2)
O5—Fe1—N2—C12	−175.0 (2)	C19—N3—C15—C16	0.4 (4)
O1—Fe1—N2—C12	−82.7 (2)	Fe2—N3—C15—C16	−171.7 (2)
O3—Fe1—N2—C12	93.0 (2)	C19—N3—C15—C20	179.8 (3)
O7—Fe1—N2—C12	1.1 (2)	Fe2—N3—C15—C20	7.7 (3)
N1—Fe1—N2—C12	139.0 (5)	N3—C15—C16—C17	−1.0 (4)
C5—N1—C1—C2	−0.1 (4)	C20—C15—C16—C17	179.6 (3)
Fe1—N1—C1—C2	−171.9 (2)	C15—C16—C17—C18	−0.4 (4)
C5—N1—C1—C6	−178.6 (3)	C16—C17—C18—C19	2.5 (4)
Fe1—N1—C1—C6	9.7 (3)	C15—N3—C19—C18	1.8 (4)
N1—C1—C2—C3	0.4 (4)	Fe2—N3—C19—C18	173.8 (2)
C6—C1—C2—C3	178.5 (3)	C15—N3—C19—C21	−173.3 (3)
C1—C2—C3—C4	−0.7 (5)	Fe2—N3—C19—C21	−1.3 (3)
C2—C3—C4—C5	0.7 (5)	C17—C18—C19—N3	−3.1 (4)
C1—N1—C5—C4	0.2 (4)	C17—C18—C19—C21	171.1 (3)
Fe1—N1—C5—C4	172.0 (2)	Fe2—O9—C20—O10	−179.9 (2)
C1—N1—C5—C7	−178.5 (3)	Fe2—O9—C20—C15	0.5 (3)
Fe1—N1—C5—C7	−6.7 (3)	N3—C15—C20—O10	175.1 (3)
C3—C4—C5—N1	−0.5 (4)	C16—C15—C20—O10	−5.6 (5)
C3—C4—C5—C7	178.0 (3)	N3—C15—C20—O9	−5.3 (4)
Fe1—O1—C6—O2	−177.1 (2)	C16—C15—C20—O9	174.1 (3)
Fe1—O1—C6—C1	0.7 (3)	Fe2—O11—C21—O12	−170.2 (2)
N1—C1—C6—O2	171.4 (3)	Fe2—O11—C21—C19	6.0 (3)
C2—C1—C6—O2	−6.9 (5)	N3—C19—C21—O12	173.4 (3)
N1—C1—C6—O1	−6.6 (4)	C18—C19—C21—O12	−1.3 (5)
C2—C1—C6—O1	175.1 (3)	N3—C19—C21—O11	−2.9 (3)
Fe1—O3—C7—O4	−170.4 (2)	C18—C19—C21—O11	−177.5 (3)
Fe1—O3—C7—C5	7.7 (3)	C26—N4—C22—C23	−0.1 (4)
N1—C5—C7—O4	177.7 (3)	Fe2—N4—C22—C23	175.0 (2)
C4—C5—C7—O4	−0.9 (5)	C26—N4—C22—C27	177.7 (3)
N1—C5—C7—O3	−0.5 (4)	Fe2—N4—C22—C27	−7.2 (3)
C4—C5—C7—O3	−179.1 (3)	N4—C22—C23—C24	0.0 (4)
C12—N2—C8—C9	0.5 (4)	C27—C22—C23—C24	−177.4 (3)
Fe1—N2—C8—C9	−174.8 (2)	C22—C23—C24—C25	0.5 (4)
C12—N2—C8—C13	176.7 (2)	C23—C24—C25—C26	−0.9 (4)

Fe1—N2—C8—C13	1.4 (3)	C22—N4—C26—C25	−0.3 (4)
N2—C8—C9—C10	0.9 (4)	Fe2—N4—C26—C25	−175.4 (2)
C13—C8—C9—C10	−174.7 (3)	C22—N4—C26—C28	178.0 (3)
C8—C9—C10—C11	−1.0 (4)	Fe2—N4—C26—C28	2.9 (3)
C9—C10—C11—C12	−0.1 (4)	C24—C25—C26—N4	0.8 (4)
C8—N2—C12—C11	−1.7 (4)	C24—C25—C26—C28	−177.2 (3)
Fe1—N2—C12—C11	173.5 (2)	Fe2—O13—C27—O14	179.1 (2)
C8—N2—C12—C14	−177.1 (3)	Fe2—O13—C27—C22	1.1 (3)
Fe1—N2—C12—C14	−1.9 (3)	N4—C22—C27—O14	−174.2 (3)
C10—C11—C12—N2	1.5 (4)	C23—C22—C27—O14	3.5 (5)
C10—C11—C12—C14	176.1 (3)	N4—C22—C27—O13	3.9 (4)
Fe1—O5—C13—O6	−177.5 (2)	C23—C22—C27—O13	−178.5 (3)
Fe1—O5—C13—C8	4.2 (3)	Fe2—O15—C28—O16	170.3 (2)
N2—C8—C13—O6	178.1 (3)	Fe2—O15—C28—C26	−7.4 (3)
C9—C8—C13—O6	−6.0 (5)	N4—C26—C28—O16	−175.1 (3)
N2—C8—C13—O5	−3.5 (4)	C25—C26—C28—O16	3.1 (5)
C9—C8—C13—O5	172.4 (3)	N4—C26—C28—O15	2.7 (4)
Fe1—O7—C14—O8	−179.2 (2)	C25—C26—C28—O15	−179.1 (3)
Fe1—O7—C14—C12	−1.1 (3)	C32—N5—C29—C30	−58.2 (3)
N2—C12—C14—O8	−180.0 (3)	C31—N6—C30—C29	−58.1 (3)
C11—C12—C14—O8	5.0 (5)	N5—C29—C30—N6	58.1 (3)
N2—C12—C14—O7	1.9 (4)	C30—N6—C31—C32	56.8 (3)
C11—C12—C14—O7	−173.1 (3)	C29—N5—C32—C31	56.7 (3)
O15—Fe2—O9—C20	−93.9 (2)	N6—C31—C32—N5	−55.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···O8	0.90	1.94	2.836 (4)	175
N5—H5B···O4^{i}	0.90	1.88	2.742 (4)	161
N6—H6A···O11	0.90	1.94	2.816 (4)	165
N6—H6B···O14^{ii}	0.90	1.84	2.738 (4)	174
O1W—H1W···O2	0.85	1.95	2.805 (4)	176
O1W—H2W···O7^{iii}	0.87	2.01	2.837 (4)	160
C4—H4A···O10^{iv}	0.93	2.31	3.221 (4)	167
C9—H9A···O6^{v}	0.93	2.28	3.103 (4)	148
C11—H11A···O15^{vi}	0.93	2.39	3.126 (4)	136
C16—H16A···O1^{vii}	0.93	2.52	3.324 (4)	144
C17—H17A···O3^{viii}	0.93	2.51	3.237 (4)	135
C18—H18A···O12^{ix}	0.93	2.45	3.234 (4)	142
C25—H25A···O16^{iv}	0.93	2.33	3.223 (4)	162
C29—H29A···O10^{x}	0.97	2.38	3.171 (4)	138
C30—H30A···O1W	0.97	2.27	3.221 (4)	167
C31—H31B···O6^{xi}	0.97	2.45	3.135 (4)	127
C32—H32A···O1W^{ii}	0.97	2.59	3.495 (4)	155
C32—H32B···O5^{xi}	0.97	2.54	3.340 (4)	140

C23—H23A···Cg4(N1/C1-C5)^{iii}	0.93	2.81	3.591 (4)	142

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

Fig. 1

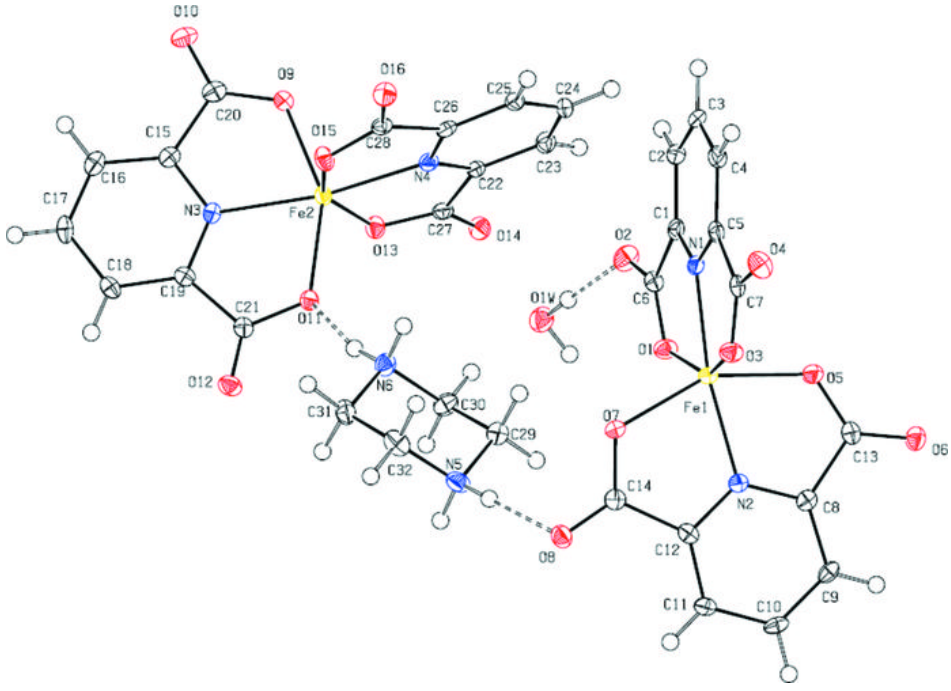
O10
O9
O16
C20
C25
C24
C26
C15
O15
C28
C3
C2
C4
C16
N4
C22
C23
C17
N3
Fe2
C1
C5
O2
N1
O4
O13
C27
O14
C18
C19
C21
O1W
C6
C7
O11
O1
O3
O5
O12
N6
Fe1
C31
C30
O7
C13
O6
C29
C32
N5
C14
N2
C8
O8
C12
C11
C10
C9

Fig. 2

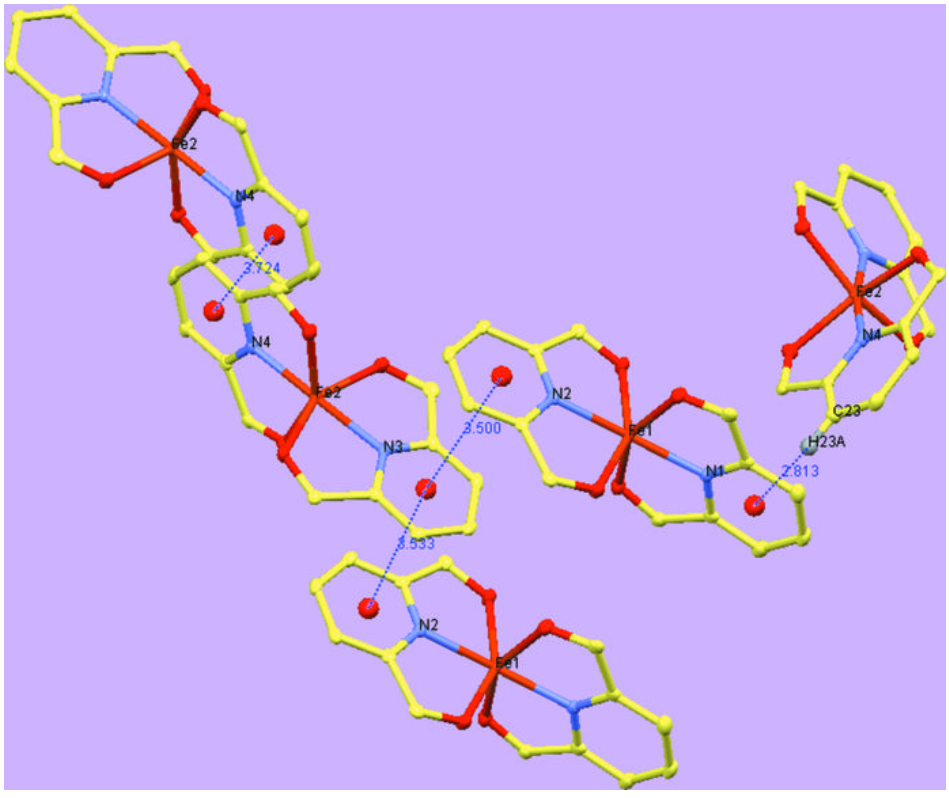
Fe2
N4
2.724
N4
Fe2
N3
3.500
3.533
N2
Fe1
N2
Fe1
N1
2.813
C23
H23A
Fe2
N4

Fig. 3