Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[(2,2′-bipyridine-κ^2N,N')-iron(II)]-μ-5-carboxy-4-carboxylato-imidazol-1-ido-$\kappa^4N^3,O^4:N^1,O^5$]

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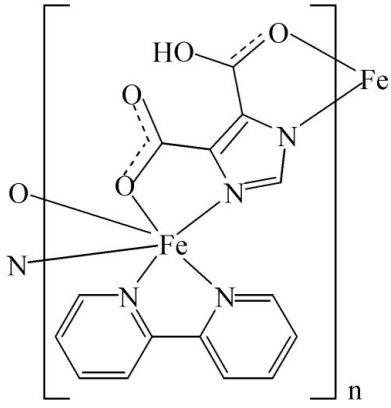
Received 9 August 2007; accepted 28 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.100; data-to-parameter ratio = 13.4.

The title compound, $[Fe(C_5H_2N_2O_4)(C_{10}H_8N_2)]_n$, was prepared by hydrothermal synthesis. The structure contains two crystallographically independent monomer units which exhibit similar geometry. The coordination environment of the Fe^{II} atom is octahedral, comprising two O atoms and four N atoms. Each Fe^{II} atom is chelated by one 2,2′-bipyridine ligand, and is linked to two neighbouring Fe^{II} atoms through bridging 5-carboxy-4-carboxylatoimidazol-1-ide ligands, forming zigzag chains parallel to the b axis. Intramolecular O—H···O hydrogen bonds are formed between the carboxy and carboxylate groups of each 5-carboxy-4-carboxylatoimidazol-1-ide ligand.

Related literature

For related literature, see: Li *et al.* (1993); Go *et al.* (2004); An *et al.* (2000); Baroni *et al.* (1996); Hundal *et al.* (2002).



Experimental

Crystal data

$[Fe(C_5H_2N_2O_4)(C_{10}H_8N_2)]$
M_r = 366.12
Monoclinic, $P2_1/c$
a = 19.9862 (10) Å
b = 9.8828 (5) Å
c = 14.4351 (7) Å
β = 101.806 (1)°
V = 2790.9 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 (2) K
0.43 × 0.35 × 0.28 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.647, T_{max} = 0.746
15091 measured reflections
5866 independent reflections
4863 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.00
5866 reflections
437 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4	0.82	1.69	2.493 (3)	167
O6—H6···O7	0.82 (3)	1.69 (2)	2.489 (2)	167 (2)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank Shandong Institute of Light Industry for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2233).

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 doi:10.1107/S1600536807042122

supplementary materials

Acta Cryst. (2007). E**63**, m2445 [**doi:10.1107/S1600536807042122**]

catena-Poly[[(2,2'-bipyridine-κ^2N,N')iron(II)]-μ-5-carboxy-4-carboxylatoimidazol-1-ido-$\kappa^4N^3,O^4:N^1,O^5$]

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Comment

Complexes containing carboxylic acids are of interest to chemists on account of their potential applications, such as catalysis, optics, information storage, medicine, molecular electrochemistry, biochemistry and biological pharmaceutics (Li *et al.*, 1993; Go *et al.*, 2004). Thus far, N-containing aromatic carboxylic acids, for example adipiodone and acetrizoic acid, have been widely used in organic synthesis, as dye intermediates, sensitization materials and functional pigments (An *et al.*, 2000). Pyridine carboxylic acid is also used extensively in coordination chemistry due to its strong coordinating ability and versatile coordination modes (Baroni *et al.* (1996); Hundal *et al.* (2002)).

In the title compound, the asymetric unit contains two crystallographically independent monomer units. As shown in Fig. 1, Fe^{II} atoms have a distorted octahedral geometry formed by two carboxylate O atoms and four N atoms, two of which belong to the 2,2'-bipyridine ligand and the other two to the imidazole ring. The Fe—O and Fe—N bond lengths are in the range 2.110 (2)–2.216 (2) and 2.071 (2)–2.296 (2) Å, respectively. The carboxy and carboxylate groups of the 5-carboxy-4-carboxylatoimidazol-1-ide ligand coordinate in a monodentate fashion to two Fe^{II} atoms, giving rise to one-dimensional zigzag chains along [010] (Fig. 2). The 2,2'-bipyridine ligands are situated between these chains.

Experimental

A mixture of $FeSO_4$ (0.1 mmol), imidazole-4,5-dicarboxylic acid (0.1 mmol) and 2,2'-bipyridine (0.1 mmol) in 10 ml of a mixed ethanol/water solvent (1:1) was placed in a 25 ml Teflon-lined stainless steel autoclave and kept at 473 K for 10 d. Green crystals of the title compound were obtained after cooling to room temperature with a yield of 5%. Elemental analysis calculated: C 49.18, H 2.73, N 7.65%; found: C 49.12, H 2.77, N 7.61%.

Refinement

H atoms bound to C atoms were placed geometrically and refined as riding atoms with C—H= 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). The H atom on O1 was also placed geometrically and refined as riding atom with O—H = 0.82 Å and with U_{iso}(H) = 1.5U_{eq}(O). The H atom on O6 was located in a difference Fourier map and refined with O—H restrained to be 0.82 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O).

Figures

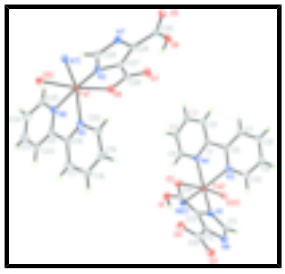

Fig. 1. The asymmetric unit of the title compound, showing displacement ellipsoids at 30% probability for non-H atoms. The suffixes I and II denote atoms generated by the symmetry operators (−*x*, *y* − 1/2, −*z* + 3/2) and (1 − *x*, *y* − 1/2, −*z* + 1/2), respectively.

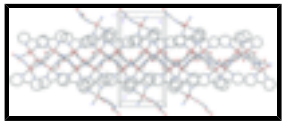

Fig. 2. Packing diagram showing zigzag chains extending palallel to [010]. H atoms have been omitted.

catena-Poly[[(2,2'-bipyridine-κ^2*N*,*N*')iron(II)]-μ- 5-carboxy-4-carboxylatoimidazol-1-*ido*- κ^4*N*^{3},*O*^{4}:*N*^{1},*O*^{5}]

Crystal data

$[Fe(C_5H_2N_2O_4)(C_{10}H_8N_2)]$	F_{000} = 1488
M_r = 366.12	D_x = 1.743 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5866 reflections
a = 19.9862 (10) Å	θ = 2.3–26.7º
b = 9.8828 (5) Å	μ = 1.11 mm^{-1}
c = 14.4351 (7) Å	*T* = 293 (2) K
β = 101.806 (1)º	Block, green
V = 2790.9 (2) Å^3	0.43 × 0.35 × 0.28 mm
Z = 8	

Data collection

Bruker APEXII CCD area-detector diffractometer	5866 independent reflections
Radiation source: fine-focus sealed tube	4863 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 26.7º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −25→20
T_{min} = 0.647, T_{max} = 0.746	*k* = −11→10
15091 measured reflections	*l* = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 2.1242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
5866 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
437 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
C1	0.25412 (13)	−0.1015 (3)	0.11260 (18)	0.0286 (6)
C2	0.18886 (14)	−0.1492 (3)	0.09414 (19)	0.0336 (6)
H2	0.1524	−0.0904	0.0745	0.040*
C3	0.17701 (14)	−0.2887 (3)	0.1050 (2)	0.0357 (6)
H3	0.1325	−0.3220	0.0911	0.043*
C4	0.23018 (15)	−0.3752 (3)	0.13573 (19)	0.0335 (6)
H4	0.2231	−0.4671	0.1437	0.040*
C5	0.29390 (14)	−0.3204 (3)	0.15413 (19)	0.0318 (6)
H5	0.3310	−0.3771	0.1754	0.038*
C6	0.27142 (13)	0.0457 (3)	0.09936 (18)	0.0287 (6)
C7	0.22341 (14)	0.1449 (3)	0.06224 (19)	0.0338 (6)
H7	0.1774	0.1219	0.0452	0.041*
C8	0.24383 (15)	0.2782 (3)	0.0504 (2)	0.0365 (6)
H8	0.2116	0.3439	0.0266	0.044*
C9	0.31112 (15)	0.3106 (3)	0.0741 (2)	0.0371 (6)
H9	0.3266	0.3978	0.0665	0.045*
C10	0.35557 (14)	0.2074 (3)	0.1101 (2)	0.0355 (6)
H10	0.4019	0.2281	0.1267	0.043*
C11	0.52108 (13)	0.1314 (3)	0.22142 (18)	0.0281 (5)
H11	0.5347	0.1320	0.1635	0.034*

C12	0.51363 (13)	0.1848 (3)	0.35977 (18)	0.0270 (5)
C13	0.47003 (13)	0.0770 (3)	0.32962 (18)	0.0265 (5)
C14	0.41974 (13)	0.0067 (3)	0.37172 (19)	0.0289 (6)
C15	0.52678 (13)	0.2659 (3)	0.44617 (18)	0.0286 (6)
C16	0.24864 (14)	−0.0084 (3)	0.85456 (18)	0.0305 (6)
C17	0.31616 (15)	0.0270 (3)	0.8779 (2)	0.0417 (7)
H17	0.3489	−0.0364	0.9043	0.050*
C18	0.33542 (16)	0.1596 (4)	0.8615 (2)	0.0486 (8)
H18	0.3814	0.1833	0.8768	0.058*
C19	0.28792 (15)	0.2557 (3)	0.8235 (2)	0.0424 (7)
H19	0.3004	0.3435	0.8115	0.051*
C20	0.22184 (14)	0.2149 (3)	0.80465 (19)	0.0342 (6)
H20	0.1882	0.2775	0.7799	0.041*
C21	0.22464 (13)	−0.1523 (3)	0.86056 (18)	0.0305 (6)
C22	0.26600 (16)	−0.2602 (3)	0.8977 (2)	0.0392 (7)
H22	0.3119	−0.2446	0.9239	0.047*
C23	0.24014 (18)	−0.3919 (3)	0.8965 (2)	0.0468 (8)
H23	0.2684	−0.4631	0.9221	0.056*
C24	0.17451 (17)	−0.4144 (3)	0.8583 (2)	0.0445 (8)
H24	0.1555	−0.5004	0.8568	0.053*
C25	0.13582 (16)	−0.3022 (3)	0.8205 (2)	0.0377 (7)
H25	0.0902	−0.3166	0.7924	0.045*
C26	0.06717 (13)	0.1530 (3)	0.60594 (17)	0.0280 (5)
C27	0.04097 (12)	0.2468 (3)	0.66939 (17)	0.0251 (5)
C28	−0.00283 (13)	0.3567 (3)	0.65276 (17)	0.0254 (5)
C29	0.02308 (13)	0.3216 (3)	0.79865 (17)	0.0267 (5)
H29	0.0255	0.3308	0.8634	0.032*
C30	−0.04275 (12)	0.4138 (3)	0.56638 (17)	0.0248 (5)
Fe1	0.100575 (14)	0.02478 (3)	0.78559 (2)	0.01296 (10)
Fe2	0.402091 (15)	−0.09584 (3)	0.18027 (2)	0.01510 (10)
N1	0.47565 (11)	0.0429 (2)	0.24137 (15)	0.0275 (5)
N2	0.05700 (11)	0.2242 (2)	0.76226 (14)	0.0265 (5)
N3	0.33654 (11)	0.0779 (2)	0.12307 (16)	0.0298 (5)
N4	0.30592 (11)	−0.1867 (2)	0.14295 (15)	0.0296 (5)
N5	0.20255 (11)	0.0867 (2)	0.82027 (15)	0.0295 (5)
N6	0.15995 (11)	−0.1735 (2)	0.82203 (16)	0.0316 (5)
N7	−0.01405 (11)	0.4035 (2)	0.73571 (14)	0.0263 (5)
N8	0.54562 (11)	0.2190 (2)	0.29037 (15)	0.0282 (5)
O1	0.41577 (10)	0.0408 (2)	0.45503 (14)	0.0355 (5)
H1	0.4462	0.0953	0.4756	0.053*
O2	0.38175 (10)	−0.0777 (2)	0.32461 (14)	0.0343 (4)
O3	0.56775 (10)	0.3637 (2)	0.45259 (13)	0.0344 (4)
O4	0.49475 (10)	0.2334 (2)	0.50895 (13)	0.0364 (5)
O5	−0.08546 (9)	0.50345 (19)	0.57110 (12)	0.0285 (4)
O6	−0.03321 (9)	0.3645 (2)	0.48931 (12)	0.0310 (4)
O7	0.05428 (11)	0.1818 (2)	0.52042 (13)	0.0394 (5)
O8	0.10133 (10)	0.0515 (2)	0.64077 (13)	0.0313 (4)
H6	−0.0001 (13)	0.314 (2)	0.499 (3)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0262 (13)	0.0346 (15)	0.0241 (12)	0.0017 (11)	0.0032 (10)	0.0001 (10)
C2	0.0277 (14)	0.0376 (16)	0.0337 (14)	−0.0009 (12)	0.0019 (11)	0.0051 (12)
C3	0.0272 (14)	0.0438 (17)	0.0343 (14)	−0.0068 (12)	0.0021 (11)	0.0025 (13)
C4	0.0366 (15)	0.0313 (15)	0.0321 (13)	−0.0073 (12)	0.0058 (11)	0.0017 (12)
C5	0.0311 (14)	0.0298 (15)	0.0337 (13)	0.0003 (11)	0.0045 (11)	0.0017 (11)
C6	0.0253 (13)	0.0333 (15)	0.0264 (12)	−0.0007 (11)	0.0029 (10)	−0.0005 (11)
C7	0.0269 (14)	0.0398 (16)	0.0326 (14)	0.0028 (12)	0.0014 (11)	0.0001 (12)
C8	0.0363 (15)	0.0330 (16)	0.0376 (15)	0.0077 (12)	0.0012 (12)	0.0046 (12)
C9	0.0390 (16)	0.0301 (15)	0.0416 (15)	−0.0019 (12)	0.0066 (13)	0.0039 (12)
C10	0.0288 (14)	0.0375 (16)	0.0393 (15)	−0.0041 (12)	0.0049 (11)	0.0021 (13)
C11	0.0240 (12)	0.0339 (15)	0.0259 (12)	−0.0025 (11)	0.0037 (10)	−0.0004 (11)
C12	0.0220 (12)	0.0312 (14)	0.0269 (12)	0.0020 (10)	0.0029 (10)	0.0012 (11)
C13	0.0232 (12)	0.0297 (14)	0.0255 (12)	0.0040 (10)	0.0025 (10)	0.0005 (10)
C14	0.0244 (13)	0.0310 (14)	0.0306 (13)	0.0036 (11)	0.0042 (10)	−0.0001 (11)
C15	0.0239 (12)	0.0309 (14)	0.0290 (13)	0.0030 (11)	0.0010 (10)	0.0001 (11)
C16	0.0258 (13)	0.0412 (16)	0.0234 (12)	0.0041 (12)	0.0028 (10)	−0.0005 (11)
C17	0.0256 (14)	0.054 (2)	0.0430 (16)	0.0045 (13)	0.0014 (12)	−0.0012 (14)
C18	0.0258 (15)	0.062 (2)	0.0547 (19)	−0.0096 (15)	0.0009 (13)	−0.0088 (17)
C19	0.0357 (16)	0.0442 (18)	0.0468 (17)	−0.0089 (14)	0.0073 (13)	−0.0026 (14)
C20	0.0318 (14)	0.0337 (16)	0.0356 (14)	−0.0034 (12)	0.0033 (11)	−0.0003 (12)
C21	0.0268 (13)	0.0417 (16)	0.0239 (12)	0.0055 (12)	0.0072 (10)	0.0032 (11)
C22	0.0341 (15)	0.0472 (19)	0.0364 (15)	0.0117 (13)	0.0076 (12)	0.0069 (13)
C23	0.0469 (19)	0.045 (2)	0.0507 (18)	0.0204 (15)	0.0159 (15)	0.0115 (15)
C24	0.0488 (19)	0.0328 (17)	0.0558 (19)	0.0067 (14)	0.0194 (16)	0.0039 (14)
C25	0.0383 (16)	0.0338 (16)	0.0441 (16)	0.0028 (13)	0.0157 (13)	0.0014 (13)
C26	0.0256 (13)	0.0311 (14)	0.0267 (12)	0.0015 (11)	0.0041 (10)	0.0007 (11)
C27	0.0220 (12)	0.0289 (14)	0.0239 (11)	−0.0013 (10)	0.0036 (9)	0.0015 (10)
C28	0.0239 (12)	0.0278 (13)	0.0243 (11)	−0.0019 (10)	0.0042 (9)	−0.0007 (10)
C29	0.0272 (13)	0.0320 (14)	0.0205 (11)	0.0009 (11)	0.0041 (9)	0.0005 (10)
C30	0.0220 (12)	0.0274 (14)	0.0247 (12)	−0.0016 (10)	0.0045 (10)	−0.0007 (10)
Fe1	0.00936 (16)	0.01382 (18)	0.01510 (16)	0.00017 (11)	0.00110 (11)	0.00294 (11)
Fe2	0.00912 (16)	0.01409 (18)	0.01998 (17)	0.00012 (11)	−0.00194 (12)	−0.00090 (12)
N1	0.0225 (11)	0.0331 (13)	0.0258 (10)	0.0005 (9)	0.0022 (8)	−0.0010 (9)
N2	0.0255 (11)	0.0296 (12)	0.0237 (10)	0.0010 (9)	0.0036 (8)	0.0018 (9)
N3	0.0246 (11)	0.0315 (12)	0.0322 (11)	−0.0007 (9)	0.0034 (9)	0.0022 (10)
N4	0.0253 (11)	0.0337 (13)	0.0282 (11)	−0.0011 (9)	0.0018 (9)	0.0008 (9)
N5	0.0233 (11)	0.0382 (14)	0.0270 (11)	0.0002 (9)	0.0049 (9)	0.0010 (9)
N6	0.0287 (12)	0.0343 (13)	0.0323 (11)	0.0042 (10)	0.0075 (9)	0.0014 (10)
N7	0.0258 (11)	0.0298 (12)	0.0227 (10)	0.0009 (9)	0.0031 (8)	−0.0003 (9)
N8	0.0251 (11)	0.0325 (12)	0.0263 (11)	−0.0008 (9)	0.0035 (8)	0.0009 (9)
O1	0.0325 (11)	0.0430 (13)	0.0332 (10)	−0.0032 (9)	0.0116 (8)	−0.0016 (9)
O2	0.0266 (10)	0.0404 (11)	0.0366 (10)	−0.0060 (8)	0.0078 (8)	−0.0017 (9)
O3	0.0307 (10)	0.0383 (11)	0.0321 (10)	−0.0033 (9)	0.0015 (8)	−0.0053 (8)
O4	0.0373 (11)	0.0437 (12)	0.0287 (10)	−0.0003 (9)	0.0078 (8)	−0.0035 (9)

O5	0.0247 (9)	0.0341 (10)	0.0259 (9)	0.0044 (8)	0.0034 (7)	0.0022 (8)
O6	0.0297 (10)	0.0377 (11)	0.0243 (9)	0.0053 (8)	0.0026 (7)	0.0014 (8)
O7	0.0485 (12)	0.0471 (13)	0.0234 (9)	0.0151 (10)	0.0089 (8)	0.0011 (9)
O8	0.0323 (10)	0.0328 (10)	0.0293 (9)	0.0077 (8)	0.0077 (8)	0.0016 (8)

Geometric parameters (Å, °)

C1—N4	1.337 (3)	C20—N5	1.357 (4)
C1—C2	1.361 (4)	C20—H20	0.930
C1—C6	1.517 (4)	C21—N6	1.316 (3)
C2—C3	1.413 (4)	C21—C22	1.388 (4)
C2—H2	0.930	C22—C23	1.400 (5)
C3—C4	1.365 (4)	C22—H22	0.930
C3—H3	0.930	C23—C24	1.333 (5)
C4—C5	1.359 (4)	C23—H23	0.930
C4—H4	0.930	C24—C25	1.397 (4)
C5—N4	1.358 (4)	C24—H24	0.930
C5—H5	0.930	C25—N6	1.358 (4)
C6—N3	1.315 (3)	C25—H25	0.930
C6—C7	1.399 (4)	C26—O7	1.241 (3)
C7—C8	1.400 (4)	C26—O8	1.259 (3)
C7—H7	0.930	C26—C27	1.473 (4)
C8—C9	1.357 (4)	C27—N2	1.332 (3)
C8—H8	0.930	C27—C28	1.384 (4)
C9—C10	1.382 (4)	C28—N7	1.345 (3)
C9—H9	0.930	C28—C30	1.450 (3)
C10—N3	1.359 (4)	C29—N7	1.325 (3)
C10—H10	0.930	C29—N2	1.345 (3)
C11—N1	1.334 (3)	C29—H29	0.930
C11—N8	1.334 (3)	C30—O5	1.242 (3)
C11—H11	0.930	C30—O6	1.264 (3)
C12—N8	1.337 (3)	Fe1—N7^{i}	2.074 (2)
C12—C13	1.389 (4)	Fe1—N5	2.088 (2)
C12—C15	1.460 (4)	Fe1—O8	2.1102 (18)
C13—N1	1.344 (3)	Fe1—N2	2.153 (2)
C13—C14	1.453 (4)	Fe1—O5^{i}	2.1613 (18)
C14—O2	1.234 (3)	Fe1—N6	2.296 (2)
C14—O1	1.267 (3)	Fe2—N1	2.071 (2)
C15—O4	1.254 (3)	Fe2—N4	2.090 (2)
C15—O3	1.258 (3)	Fe2—N8^{ii}	2.107 (2)
C16—N5	1.338 (4)	Fe2—O3^{ii}	2.162 (2)
C16—C17	1.368 (4)	Fe2—O2	2.210 (2)
C16—C21	1.509 (4)	Fe2—N3	2.215 (2)
C17—C18	1.399 (5)	N7—Fe1^{iii}	2.074 (2)
C17—H17	0.930	N8—Fe2^{iv}	2.107 (2)
C18—C19	1.375 (5)	O1—H1	0.820
C18—H18	0.930	O3—Fe2^{iv}	2.162 (2)

C19—C20	1.354 (4)	O5—Fe1^{iii}	2.1613 (18)
C19—H19	0.930	O6—H6	0.82 (3)
N4—C1—C2	119.5 (3)	O7—C26—O8	124.4 (2)
N4—C1—C6	117.7 (2)	O7—C26—C27	116.5 (2)
C2—C1—C6	122.8 (2)	O8—C26—C27	119.1 (2)
C1—C2—C3	119.5 (3)	N2—C27—C28	108.6 (2)
C1—C2—H2	120.3	N2—C27—C26	118.5 (2)
C3—C2—H2	120.3	C28—C27—C26	132.7 (2)
C4—C3—C2	120.7 (3)	N7—C28—C27	109.3 (2)
C4—C3—H3	119.7	N7—C28—C30	118.0 (2)
C2—C3—H3	119.7	C27—C28—C30	132.2 (2)
C5—C4—C3	116.8 (3)	N7—C29—N2	115.2 (2)
C5—C4—H4	121.6	N7—C29—H29	122.4
C3—C4—H4	121.6	N2—C29—H29	122.4
N4—C5—C4	123.1 (3)	O5—C30—O6	123.5 (2)
N4—C5—H5	118.5	O5—C30—C28	119.6 (2)
C4—C5—H5	118.5	O6—C30—C28	116.8 (2)
N3—C6—C7	119.7 (3)	N7^{i}—Fe1—N5	161.40 (9)
N3—C6—C1	116.0 (2)	N7^{i}—Fe1—O8	95.75 (8)
C7—C6—C1	124.3 (2)	N5—Fe1—O8	89.80 (8)
C6—C7—C8	120.8 (3)	N7^{i}—Fe1—N2	101.96 (8)
C6—C7—H7	119.6	N5—Fe1—N2	96.50 (9)
C8—C7—H7	119.6	O8—Fe1—N2	79.36 (8)
C9—C8—C7	119.4 (3)	N7^{i}—Fe1—O5^{i}	79.05 (7)
C9—C8—H8	120.3	N5—Fe1—O5^{i}	96.88 (8)
C7—C8—H8	120.3	O8—Fe1—O5^{i}	172.39 (7)
C8—C9—C10	116.6 (3)	N2—Fe1—O5^{i}	96.18 (7)
C8—C9—H9	121.7	N7^{i}—Fe1—N6	85.24 (8)
C10—C9—H9	121.7	N5—Fe1—N6	76.21 (9)
N3—C10—C9	124.7 (3)	O8—Fe1—N6	103.04 (8)
N3—C10—H10	117.6	N2—Fe1—N6	172.23 (8)
C9—C10—H10	117.6	O5^{i}—Fe1—N6	82.20 (8)
N1—C11—N8	115.3 (2)	N1—Fe2—N4	158.38 (9)
N1—C11—H11	122.4	N1—Fe2—N8^{ii}	102.12 (8)
N8—C11—H11	122.4	N4—Fe2—N8^{ii}	94.04 (9)
N8—C12—C13	108.9 (2)	N1—Fe2—O3^{ii}	101.41 (8)
N8—C12—C15	118.1 (2)	N4—Fe2—O3^{ii}	95.76 (8)
C13—C12—C15	132.9 (2)	N8^{ii}—Fe2—O3^{ii}	78.51 (8)
N1—C13—C12	108.7 (2)	N1—Fe2—O2	78.24 (8)
N1—C13—C14	118.4 (2)	N4—Fe2—O2	86.62 (8)
C12—C13—C14	132.8 (2)	N8^{ii}—Fe2—O2	93.45 (8)
O2—C14—O1	123.5 (3)	O3^{ii}—Fe2—O2	171.74 (7)
O2—C14—C13	119.5 (2)	N1—Fe2—N3	87.68 (8)
O1—C14—C13	116.9 (2)	N4—Fe2—N3	78.15 (9)
O4—C15—O3	124.4 (2)	N8^{ii}—Fe2—N3	168.44 (8)

O4—C15—C12	116.6 (2)	O3^{ii}—Fe2—N3	93.66 (8)
O3—C15—C12	119.0 (2)	O2—Fe2—N3	94.57 (8)
N5—C16—C17	118.8 (3)	C11—N1—C13	103.5 (2)
N5—C16—C21	118.7 (2)	C11—N1—Fe2	142.88 (18)
C17—C16—C21	122.4 (3)	C13—N1—Fe2	112.30 (17)
C16—C17—C18	119.3 (3)	C27—N2—C29	103.7 (2)
C16—C17—H17	120.3	C27—N2—Fe1	108.53 (17)
C18—C17—H17	120.3	C29—N2—Fe1	144.53 (17)
C19—C18—C17	121.5 (3)	C6—N3—C10	118.8 (2)
C19—C18—H18	119.2	C6—N3—Fe2	112.81 (18)
C17—C18—H18	119.2	C10—N3—Fe2	128.37 (18)
C20—C19—C18	116.1 (3)	C1—N4—C5	120.5 (2)
C20—C19—H19	122.0	C1—N4—Fe2	115.04 (18)
C18—C19—H19	122.0	C5—N4—Fe2	124.28 (18)
C19—C20—N5	122.9 (3)	C16—N5—C20	121.3 (2)
C19—C20—H20	118.5	C16—N5—Fe1	116.59 (19)
N5—C20—H20	118.5	C20—N5—Fe1	122.02 (18)
N6—C21—C22	119.8 (3)	C21—N6—C25	118.1 (2)
N6—C21—C16	115.0 (2)	C21—N6—Fe1	112.18 (19)
C22—C21—C16	125.1 (3)	C25—N6—Fe1	129.06 (19)
C21—C22—C23	121.4 (3)	C29—N7—C28	103.2 (2)
C21—C22—H22	119.3	C29—N7—Fe1^{iii}	141.96 (18)
C23—C22—H22	119.3	C28—N7—Fe1^{iii}	110.65 (16)
C24—C23—C22	119.3 (3)	C11—N8—C12	103.6 (2)
C24—C23—H23	120.3	C11—N8—Fe2^{iv}	143.60 (18)
C22—C23—H23	120.3	C12—N8—Fe2^{iv}	111.23 (17)
C23—C24—C25	116.6 (3)	C14—O1—H1	109.5
C23—C24—H24	121.7	C14—O2—Fe2	111.30 (17)
C25—C24—H24	121.7	C15—O3—Fe2^{iv}	111.86 (16)
N6—C25—C24	124.8 (3)	C30—O5—Fe1^{iii}	110.75 (15)
N6—C25—H25	117.6	C30—O6—H6	110 (3)
C24—C25—H25	117.6	C26—O8—Fe1	112.45 (16)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4	0.82	1.69	2.493 (3)	167
O6—H6···O7	0.82 (3)	1.69 (2)	2.489 (2)	167 (2)

Fig. 1

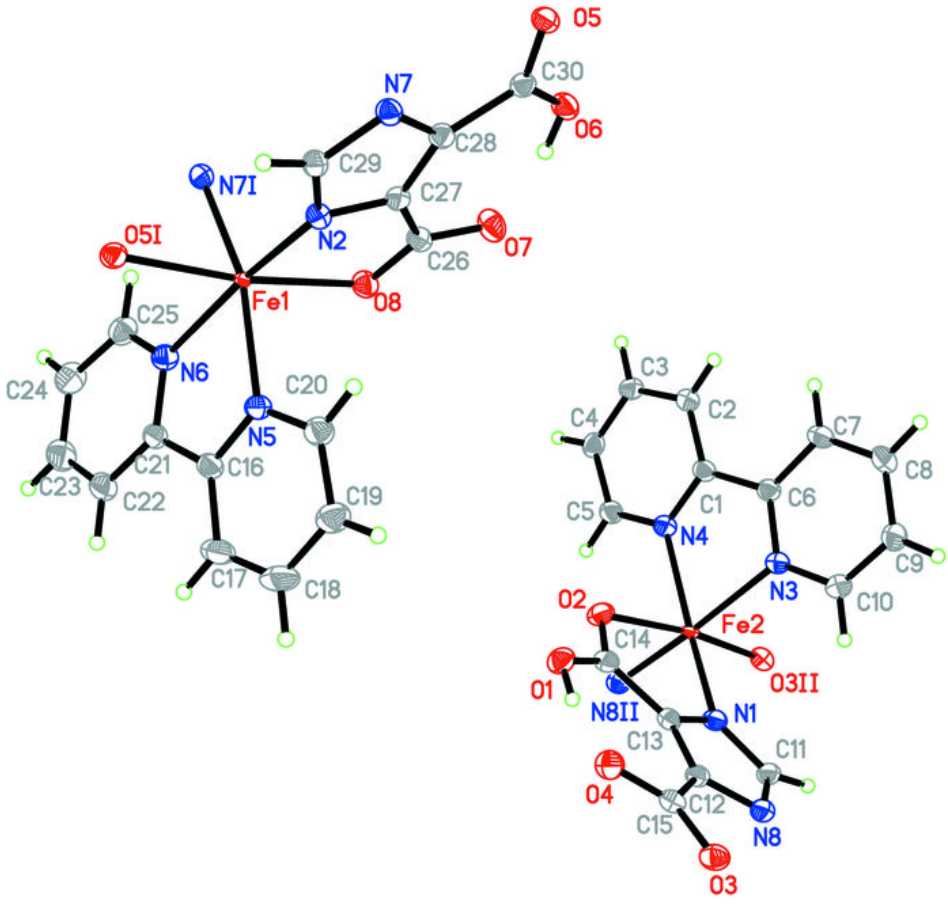
O5
C30
N7
O6
C28
C29
N7I
C27
N2
O5I
O7
C26
Fe1
O8
C25
N6
C24
C20
N5
C21
C16
C23
C22
C19
C17
C18
C3
C4
C2
C7
C8
C5
C1
C6
N4
C9
N3
C10
O2
Fe2
C14
O1
O3II
N8II
N1
C13
C11
O4
C12
C15
N8
O3

Fig. 2