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Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate

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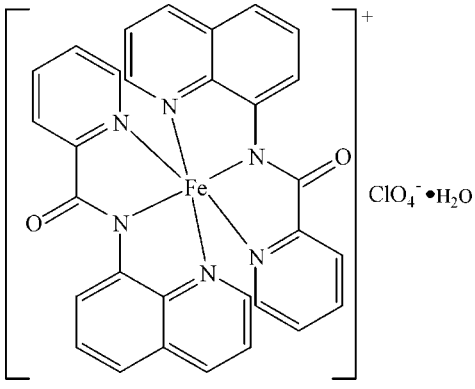
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.054; wR factor = 0.140; data-to-parameter ratio = 13.5.

The asymmetric unit of the title compound, $[Fe(C_{15}H_{10}N_3O)_2]ClO_4\cdot H_2O$, contains one iron(III) cation chelated by two *N*-(8-naphthyl)-2-pyridine-2-carboxamidate ligands *via* six N atoms, exhibiting an octahedral coordination geometry, a perchlorate anion and a water molecule. The Fe—N bond lengths are in the range 1.880 (3)–1.972 (3) Å. Each ligand is planar (r.m.s. deviations = 0.0314 and 0.0282 Å). The dihedral angle between the two ligand planes is 86.55 (1)°. There is a weak intermolecular hydrogen bond between the water and the perchlorate groups.

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

$[Fe(C_{15}H_{10}N_3O)_2]ClO_4\cdot H_2O$
M_r = 669.84
Triclinic, $P\overline{1}$
a = 9.2452 (10) Å
b = 11.944 (2) Å
c = 13.0523 (10) Å
α = 95.807 (5)°
β = 90.462 (1)°
γ = 91.615 (5)°
V = 1433.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 293 (2) K
0.42 × 0.26 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.763, T_{max} = 0.865
13425 measured reflections
5559 independent reflections
3729 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.140
S = 1.00
5559 reflections
413 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O4^{i}	0.84 (3)	2.25 (4)	2.934 (12)	139 (4)

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

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2152).

References

An, J., Chen, Z. D., Bian, J., Chen, J. T., Wang, S. X., Gao, S. & Xu, G. X. (2000). *Inorg. Chim. Acta*, **299**, 28–30.
Baroni, T. E., Heppert, J. A., Hodel, R. R., Kingsborough, R. P., Morton, M. D., Pheingold, A. L. & Yap, G. P. A. (1996). *Organometallics*, **15**, 4872–4874.
Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Go, Y. B., Wang, X. Q. & Anokhina, E. V. (2004). *Inorg. Chem.* **43**, 5360–5364.
Hundal, G., Hundal, M. S., Obrai, S., Poonia, N. S. & Kumar, S. (2002). *Inorg. Chem.* **41**, 2077–2086.
Li, M. X., Xu, Z. & You, X. Z. (1993). *Polyhedron*, **12**, 921–923.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate

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Comment

Complexes containing carbonyl amine (organic amide) ligands have been the interest of chemists due to their potential applications, such as in catalysis, optics, information storage, medicine, molecular electrochemistry, biochemistry and biological pharmaceuticals (Li *et al.*, 1993; Go *et al.*, 2004). Thus far, N-containing aromatic carbonyl amines have been widely used in dye intermediates, organic synthesis, sensitization materials, functional pigments, adipiodone and acetrizoic acid (An *et al.*, 2000). Pyridine carbonyl amine is also a good ligand in coordination chemistry due to its strong coordination ability and versatile coordination modes, so much attention has been paid to it in recent years (Baroni *et al.*, 1996; Hundal *et al.*, 2002). Here we report the new title complex.

The title compound contains an iron(III) cation chelated by two 2-pyridinecarbonyl-8-aminoquinoline ligands *via* six N atoms, exhibiting octahedral geometry around the central iron ion (Fig. 1). The Fe—N bond length are in the range 1.880 (3)–1.972 (3) Å. Each ligand is planar (r.m.s. deviations 0.0314 and 0.0282 Å). The dihedral angle between the two ligand planes is 86.55 (1)°. There is a weak intermolecular hydrogen bond between water and perchlorate, contributing to the packing.

Experimental

A mixture of iron trichloride (0.1 mmol) and 2-pyridinecarbonyl-8-aminoquinoline (0.2 mmol) in 25 ml me thanol was refluxed for 2 h and filtered. The filtrate was evaporated naturally in an open flask. Green crystals were obtained after one week in a yield of 12%. Anal. Calc. for $C_{30}H_{22}ClFeN_6O_7$: C 53.73, H 2.99, N 12.54%; Found: 53.68, H 3.02, N 12.51%.

Refinement

The H atoms of the water molecule were located in a difference density map and were refined with distance restraints [H···H = 1.38 (2) Å and O—H = 0.82 (2) Å] and with U_{iso}(H) = 0.08 Å^2. All other H atoms were placed in calculated positions with a C—H bond distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

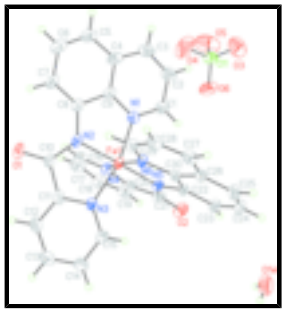


Fig. 1. The asymmetric unit of the title structure, drawn with 30% probability displacement ellipsoids.

Bis[*N*-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate

Crystal data

$[Fe(C_{15}H_{10}N_3O)_2]ClO_4·H_2O$	$Z = 2$
$M_r = 669.84$	$F_{000} = 686$
Triclinic, $P\overline{1}$	$D_x = 1.552$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.2452$ (10) Å	Cell parameters from 5559 reflections
$b = 11.944$ (2) Å	$\theta = 3.1$–26.0º
$c = 13.0523$ (10) Å	$\mu = 0.68$ mm^{-1}
$\alpha = 95.807$ (5)º	$T = 293$ (2) K
$\beta = 90.462$ (1)º	Block, green
$\gamma = 91.615$ (5)º	0.42 × 0.26 × 0.22 mm
$V = 1433.3$ (3) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	5559 independent reflections
Radiation source: fine-focus sealed tube	3729 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 293$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 3.1$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = 0 \rightarrow 11$
$T_{min} = 0.763$, $T_{max} = 0.865$	$k = -14 \rightarrow 14$
13425 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.140$	$w = 1/[\sigma^2(F_o^2) + (0.092P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
5559 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
413 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
3 restraints	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 $F^2 > 2\text{sigma}(F^2)$ 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	0.7506 (5)	0.3112 (4)	0.3721 (3)	0.0659 (10)
H1A	0.7130	0.3810	0.3939	0.079*
C2	0.8893 (6)	0.2844 (5)	0.4060 (4)	0.0892 (15)
H2A	0.9414	0.3358	0.4515	0.107*
C3	0.9464 (5)	0.1862 (5)	0.3735 (4)	0.0820 (13)
H3A	1.0389	0.1704	0.3954	0.098*
C4	0.8682 (5)	0.1051 (4)	0.3056 (3)	0.0654 (11)
C5	0.9158 (5)	−0.0009 (5)	0.2647 (4)	0.0792 (13)
H5A	1.0073	−0.0234	0.2826	0.095*
C6	0.8324 (6)	−0.0699 (4)	0.2007 (4)	0.0796 (14)
H6A	0.8677	−0.1392	0.1751	0.096*
C7	0.6920 (5)	−0.0408 (3)	0.1706 (3)	0.0628 (10)
H7A	0.6361	−0.0905	0.1261	0.075*
C8	0.6395 (4)	0.0610 (3)	0.2073 (3)	0.0499 (8)
C9	0.7297 (4)	0.1362 (3)	0.2760 (3)	0.0493 (8)
C10	0.3957 (4)	0.0540 (3)	0.1333 (3)	0.0565 (9)
C11	0.2748 (4)	0.1304 (3)	0.1266 (3)	0.0558 (9)
C12	0.1473 (5)	0.1020 (4)	0.0708 (4)	0.0775 (13)
H12A	0.1345	0.0310	0.0349	0.093*
C13	0.0417 (6)	0.1792 (5)	0.0691 (5)	0.0886 (15)
H13A	−0.0438	0.1605	0.0325	0.106*
C14	0.0606 (5)	0.2840 (4)	0.1211 (4)	0.0719 (11)
H14A	−0.0106	0.3373	0.1190	0.086*

C15	0.1869 (4)	0.3094 (3)	0.1767 (3)	0.0549 (8)
H15A	0.1990	0.3798	0.2139	0.066*
C16	0.3662 (4)	0.1163 (4)	0.4101 (3)	0.0652 (10)
H16A	0.3955	0.0529	0.3692	0.078*
C17	0.2985 (5)	0.1049 (5)	0.5041 (4)	0.0806 (14)
H17A	0.2844	0.0338	0.5262	0.097*
C18	0.2533 (5)	0.1969 (5)	0.5631 (3)	0.0823 (14)
H18A	0.2067	0.1890	0.6249	0.099*
C19	0.2761 (4)	0.3008 (4)	0.5316 (3)	0.0672 (11)
H19A	0.2458	0.3645	0.5717	0.081*
C20	0.3443 (4)	0.3107 (3)	0.4402 (2)	0.0523 (8)
C21	0.3797 (4)	0.4214 (3)	0.4006 (3)	0.0527 (8)
C22	0.5049 (4)	0.4906 (3)	0.2525 (3)	0.0466 (7)
C23	0.4968 (5)	0.6065 (3)	0.2745 (3)	0.0617 (10)
H23A	0.4490	0.6370	0.3327	0.074*
C24	0.5625 (5)	0.6769 (3)	0.2070 (4)	0.0744 (12)
H24A	0.5569	0.7544	0.2219	0.089*
C25	0.6329 (5)	0.6370 (3)	0.1220 (4)	0.0709 (12)
H25A	0.6763	0.6868	0.0804	0.085*
C26	0.6412 (4)	0.5202 (3)	0.0953 (3)	0.0583 (9)
C27	0.7120 (4)	0.4666 (4)	0.0094 (3)	0.0629 (10)
H27A	0.7621	0.5101	−0.0346	0.075*
C28	0.7083 (4)	0.3521 (4)	−0.0105 (3)	0.0625 (10)
H28A	0.7535	0.3176	−0.0683	0.075*
C29	0.6363 (4)	0.2882 (3)	0.0567 (3)	0.0528 (8)
H29A	0.6335	0.2103	0.0423	0.063*
C30	0.5729 (4)	0.4481 (3)	0.1621 (3)	0.0467 (7)
Cl1	0.98024 (13)	0.38673 (11)	0.75442 (12)	0.0874 (4)
Fe1	0.48026 (5)	0.25820 (4)	0.25203 (3)	0.03984 (17)
N1	0.6730 (3)	0.2379 (2)	0.3095 (2)	0.0500 (7)
N2	0.5060 (3)	0.1068 (2)	0.1892 (2)	0.0493 (7)
N3	0.2932 (3)	0.2345 (2)	0.1783 (2)	0.0439 (6)
N4	0.3889 (3)	0.2191 (2)	0.3789 (2)	0.0478 (6)
N5	0.4503 (3)	0.4062 (2)	0.3099 (2)	0.0448 (6)
N6	0.5710 (3)	0.3329 (2)	0.1409 (2)	0.0437 (6)
O1	0.3877 (4)	−0.0438 (2)	0.0916 (3)	0.0865 (10)
O2	0.3503 (4)	0.5108 (3)	0.4477 (2)	0.0778 (8)
O3	1.0848 (7)	0.4603 (6)	0.7251 (5)	0.166 (2)
O4	0.9827 (10)	0.2839 (6)	0.6934 (8)	0.227 (4)
O5	1.0194 (7)	0.3498 (9)	0.8547 (6)	0.217 (4)
O6	0.8419 (5)	0.4240 (4)	0.7667 (4)	0.1305 (16)
O1W	0.2728 (13)	0.8676 (9)	0.3076 (14)	0.131 (3)
H1W	0.205 (4)	0.839 (4)	0.339 (3)	0.080*
H2W	0.265 (5)	0.846 (5)	0.2461 (12)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.065 (2)	0.067 (2)	0.062 (2)	0.0114 (19)	−0.0079 (19)	−0.0116 (19)
C2	0.071 (3)	0.103 (4)	0.089 (4)	0.007 (3)	−0.023 (2)	−0.015 (3)
C3	0.065 (3)	0.101 (4)	0.081 (3)	0.016 (3)	−0.013 (2)	0.010 (3)
C4	0.068 (2)	0.073 (3)	0.061 (2)	0.024 (2)	0.0157 (19)	0.029 (2)
C5	0.072 (3)	0.082 (3)	0.089 (3)	0.028 (2)	0.013 (2)	0.026 (3)
C6	0.098 (4)	0.065 (3)	0.081 (3)	0.030 (3)	0.033 (3)	0.023 (2)
C7	0.080 (3)	0.0421 (18)	0.068 (2)	0.0120 (17)	0.019 (2)	0.0127 (17)
C8	0.065 (2)	0.0432 (17)	0.0430 (18)	0.0080 (15)	0.0105 (15)	0.0080 (14)
C9	0.059 (2)	0.0482 (18)	0.0431 (18)	0.0130 (15)	0.0152 (14)	0.0123 (14)
C10	0.069 (2)	0.0368 (17)	0.061 (2)	−0.0049 (16)	0.0072 (18)	−0.0056 (15)
C11	0.063 (2)	0.0456 (18)	0.057 (2)	−0.0090 (16)	0.0050 (16)	−0.0014 (15)
C12	0.074 (3)	0.067 (3)	0.086 (3)	−0.015 (2)	−0.007 (2)	−0.016 (2)
C13	0.069 (3)	0.087 (3)	0.106 (4)	−0.001 (3)	−0.019 (3)	−0.005 (3)
C14	0.058 (2)	0.080 (3)	0.078 (3)	0.005 (2)	−0.007 (2)	0.010 (2)
C15	0.060 (2)	0.053 (2)	0.053 (2)	0.0063 (16)	0.0018 (16)	0.0094 (16)
C16	0.063 (2)	0.078 (3)	0.058 (2)	0.003 (2)	0.0010 (18)	0.023 (2)
C17	0.082 (3)	0.101 (4)	0.064 (3)	−0.007 (3)	0.007 (2)	0.035 (3)
C18	0.075 (3)	0.128 (5)	0.045 (2)	−0.004 (3)	0.014 (2)	0.016 (3)
C19	0.064 (2)	0.096 (3)	0.041 (2)	0.005 (2)	0.0107 (16)	0.001 (2)
C20	0.0500 (19)	0.072 (2)	0.0333 (16)	0.0063 (16)	−0.0027 (13)	−0.0014 (15)
C21	0.055 (2)	0.057 (2)	0.0434 (18)	0.0195 (16)	−0.0027 (15)	−0.0150 (15)
C22	0.0518 (19)	0.0366 (16)	0.0495 (19)	0.0031 (13)	−0.0073 (14)	−0.0048 (13)
C23	0.070 (2)	0.0432 (18)	0.069 (3)	0.0068 (17)	−0.0058 (19)	−0.0076 (17)
C24	0.086 (3)	0.0384 (19)	0.099 (4)	−0.0039 (19)	−0.010 (3)	0.010 (2)
C25	0.075 (3)	0.051 (2)	0.088 (3)	−0.015 (2)	−0.008 (2)	0.021 (2)
C26	0.054 (2)	0.053 (2)	0.069 (2)	−0.0122 (17)	−0.0141 (17)	0.0205 (18)
C27	0.056 (2)	0.079 (3)	0.057 (2)	−0.0057 (19)	0.0038 (17)	0.027 (2)
C28	0.058 (2)	0.081 (3)	0.050 (2)	0.0023 (19)	0.0108 (16)	0.0108 (19)
C29	0.055 (2)	0.054 (2)	0.0493 (19)	0.0042 (15)	0.0015 (15)	0.0044 (16)
C30	0.0432 (17)	0.0452 (17)	0.0511 (19)	−0.0048 (14)	−0.0085 (14)	0.0033 (14)
Cl1	0.0700 (7)	0.0850 (8)	0.1068 (10)	0.0213 (6)	0.0178 (6)	0.0009 (7)
Fe1	0.0500 (3)	0.0338 (2)	0.0350 (3)	0.00393 (17)	0.00660 (17)	−0.00136 (17)
N1	0.0540 (16)	0.0532 (16)	0.0425 (15)	−0.0015 (13)	0.0048 (12)	0.0040 (12)
N2	0.0642 (18)	0.0317 (13)	0.0509 (16)	0.0042 (12)	0.0100 (13)	−0.0018 (11)
N3	0.0504 (15)	0.0390 (13)	0.0419 (14)	−0.0029 (11)	0.0076 (11)	0.0028 (11)
N4	0.0561 (16)	0.0530 (16)	0.0354 (14)	0.0044 (13)	0.0022 (11)	0.0096 (12)
N5	0.0513 (16)	0.0417 (14)	0.0408 (14)	0.0076 (12)	0.0022 (11)	−0.0013 (11)
N6	0.0530 (15)	0.0378 (13)	0.0392 (14)	−0.0006 (11)	0.0033 (11)	−0.0011 (11)
O1	0.100 (2)	0.0401 (14)	0.113 (3)	−0.0018 (15)	−0.0040 (19)	−0.0202 (15)
O2	0.099 (2)	0.0683 (18)	0.0624 (17)	0.0251 (15)	0.0108 (15)	−0.0191 (14)
O3	0.149 (5)	0.175 (6)	0.180 (6)	−0.043 (4)	0.034 (4)	0.052 (5)
O4	0.264 (9)	0.114 (5)	0.294 (10)	0.041 (5)	0.111 (7)	−0.046 (5)
O5	0.143 (5)	0.369 (12)	0.157 (6)	0.035 (6)	0.007 (4)	0.110 (7)
O6	0.107 (3)	0.134 (4)	0.157 (4)	0.057 (3)	0.024 (3)	0.027 (3)
O1W	0.188 (9)	0.117 (6)	0.088 (6)	0.054 (6)	0.041 (5)	−0.008 (5)

Geometric parameters (Å, °)

C1—N1	1.327 (5)	C18—H18A	0.930

C1—C2	1.410 (6)	C19—C20	1.368 (5)
C1—H1A	0.930	C19—H19A	0.930
C2—C3	1.332 (7)	C20—N4	1.363 (5)
C2—H2A	0.930	C20—C21	1.496 (6)
C3—C4	1.422 (7)	C21—O2	1.215 (4)
C3—H3A	0.930	C21—N5	1.356 (4)
C4—C5	1.407 (7)	C22—C23	1.389 (5)
C4—C9	1.406 (6)	C22—C30	1.398 (5)
C5—C6	1.336 (8)	C22—N5	1.400 (4)
C5—H5A	0.930	C23—C24	1.408 (6)
C6—C7	1.416 (7)	C23—H23A	0.930
C6—H6A	0.930	C24—C25	1.343 (7)
C7—C8	1.365 (5)	C24—H24A	0.930
C7—H7A	0.930	C25—C26	1.408 (6)
C8—N2	1.392 (5)	C25—H25A	0.930
C8—C9	1.445 (5)	C26—C27	1.409 (6)
C9—N1	1.368 (5)	C26—C30	1.424 (5)
C10—O1	1.239 (4)	C27—C28	1.366 (6)
C10—N2	1.352 (5)	C27—H27A	0.930
C10—C11	1.470 (6)	C28—C29	1.381 (5)
C11—N3	1.359 (4)	C28—H28A	0.930
C11—C12	1.396 (6)	C29—N6	1.330 (5)
C12—C13	1.363 (7)	C29—H29A	0.930
C12—H12A	0.930	C30—N6	1.376 (4)
C13—C14	1.368 (7)	Cl1—O3	1.371 (5)
C13—H13A	0.930	Cl1—O6	1.372 (4)
C14—C15	1.380 (6)	Cl1—O4	1.395 (7)
C14—H14A	0.930	Cl1—O5	1.469 (7)
C15—N3	1.349 (5)	Fe1—N5	1.880 (3)
C15—H15A	0.930	Fe1—N2	1.930 (3)
C16—N4	1.343 (5)	Fe1—N1	1.959 (3)
C16—C17	1.400 (6)	Fe1—N4	1.958 (3)
C16—H16A	0.930	Fe1—N6	1.960 (3)
C17—C18	1.355 (8)	Fe1—N3	1.972 (3)
C17—H17A	0.930	O1W—H1W	0.84 (3)
C18—C19	1.357 (7)	O1W—H2W	0.82 (3)
N1—C1—C2	120.6 (4)	C30—C22—N5	113.1 (3)
N1—C1—H1A	119.7	C22—C23—C24	118.8 (4)
C2—C1—H1A	119.7	C22—C23—H23A	120.6
C3—C2—C1	120.5 (5)	C24—C23—H23A	120.6
C3—C2—H2A	119.7	C25—C24—C23	122.9 (4)
C1—C2—H2A	119.7	C25—C24—H24A	118.6
C2—C3—C4	121.0 (4)	C23—C24—H24A	118.6
C2—C3—H3A	119.5	C24—C25—C26	120.4 (4)
C4—C3—H3A	119.5	C24—C25—H25A	119.8
C5—C4—C9	117.4 (4)	C26—C25—H25A	119.8
C5—C4—C3	126.9 (4)	C27—C26—C25	126.5 (4)
C9—C4—C3	115.7 (4)	C27—C26—C30	116.3 (3)
C6—C5—C4	121.5 (5)	C25—C26—C30	117.2 (4)

C6—C5—H5A	119.3	C28—C27—C26	121.2 (4)
C4—C5—H5A	119.3	C28—C27—H27A	119.4
C5—C6—C7	122.1 (4)	C26—C27—H27A	119.4
C5—C6—H6A	119.0	C27—C28—C29	118.9 (4)
C7—C6—H6A	119.0	C27—C28—H28A	120.5
C8—C7—C6	119.4 (4)	C29—C28—H28A	120.5
C8—C7—H7A	120.3	N6—C29—C28	123.1 (4)
C6—C7—H7A	120.3	N6—C29—H29A	118.5
C7—C8—N2	129.4 (4)	C28—C29—H29A	118.5
C7—C8—C9	118.7 (4)	N6—C30—C22	116.6 (3)
N2—C8—C9	111.8 (3)	N6—C30—C26	121.5 (3)
N1—C9—C4	122.6 (4)	C22—C30—C26	121.9 (3)
N1—C9—C8	116.5 (3)	O3—Cl1—O6	118.2 (4)
C4—C9—C8	120.9 (3)	O3—Cl1—O4	111.2 (5)
O1—C10—N2	128.8 (4)	O6—Cl1—O4	111.5 (5)
O1—C10—C11	120.9 (4)	O3—Cl1—O5	109.7 (5)
N2—C10—C11	110.3 (3)	O6—Cl1—O5	104.6 (4)
N3—C11—C12	120.0 (4)	O4—Cl1—O5	99.8 (6)
N3—C11—C10	116.0 (3)	N5—Fe1—N2	178.08 (13)
C12—C11—C10	124.1 (3)	N5—Fe1—N1	98.93 (12)
C13—C12—C11	119.5 (4)	N2—Fe1—N1	82.88 (12)
C13—C12—H12A	120.3	N5—Fe1—N4	83.05 (12)
C11—C12—H12A	120.3	N2—Fe1—N4	97.59 (12)
C12—C13—C14	120.4 (4)	N1—Fe1—N4	91.11 (12)
C12—C13—H13A	119.8	N5—Fe1—N6	83.80 (11)
C14—C13—H13A	119.8	N2—Fe1—N6	95.61 (11)
C13—C14—C15	118.9 (4)	N1—Fe1—N6	89.06 (12)
C13—C14—H14A	120.5	N4—Fe1—N6	166.71 (11)
C15—C14—H14A	120.5	N5—Fe1—N3	97.17 (12)
N3—C15—C14	121.4 (4)	N2—Fe1—N3	81.03 (12)
N3—C15—H15A	119.3	N1—Fe1—N3	163.89 (12)
C14—C15—H15A	119.3	N4—Fe1—N3	90.17 (11)
N4—C16—C17	119.9 (4)	N6—Fe1—N3	93.34 (11)
N4—C16—H16A	120.0	C1—N1—C9	119.6 (3)
C17—C16—H16A	120.0	C1—N1—Fe1	127.3 (3)
C18—C17—C16	120.2 (5)	C9—N1—Fe1	113.1 (2)
C18—C17—H17A	119.9	C10—N2—C8	125.6 (3)
C16—C17—H17A	119.9	C10—N2—Fe1	118.8 (2)
C19—C18—C17	119.8 (4)	C8—N2—Fe1	115.6 (2)
C19—C18—H18A	120.1	C15—N3—C11	119.7 (3)
C17—C18—H18A	120.1	C15—N3—Fe1	126.5 (2)
C18—C19—C20	119.2 (4)	C11—N3—Fe1	113.8 (2)
C18—C19—H19A	120.4	C16—N4—C20	118.8 (3)
C20—C19—H19A	120.4	C16—N4—Fe1	128.1 (3)
N4—C20—C19	122.0 (4)	C20—N4—Fe1	113.1 (2)
N4—C20—C21	114.7 (3)	C21—N5—C22	126.6 (3)
C19—C20—C21	123.4 (4)	C21—N5—Fe1	118.4 (2)
O2—C21—N5	126.8 (4)	C22—N5—Fe1	115.0 (2)
O2—C21—C20	122.5 (3)	C29—N6—C30	118.9 (3)

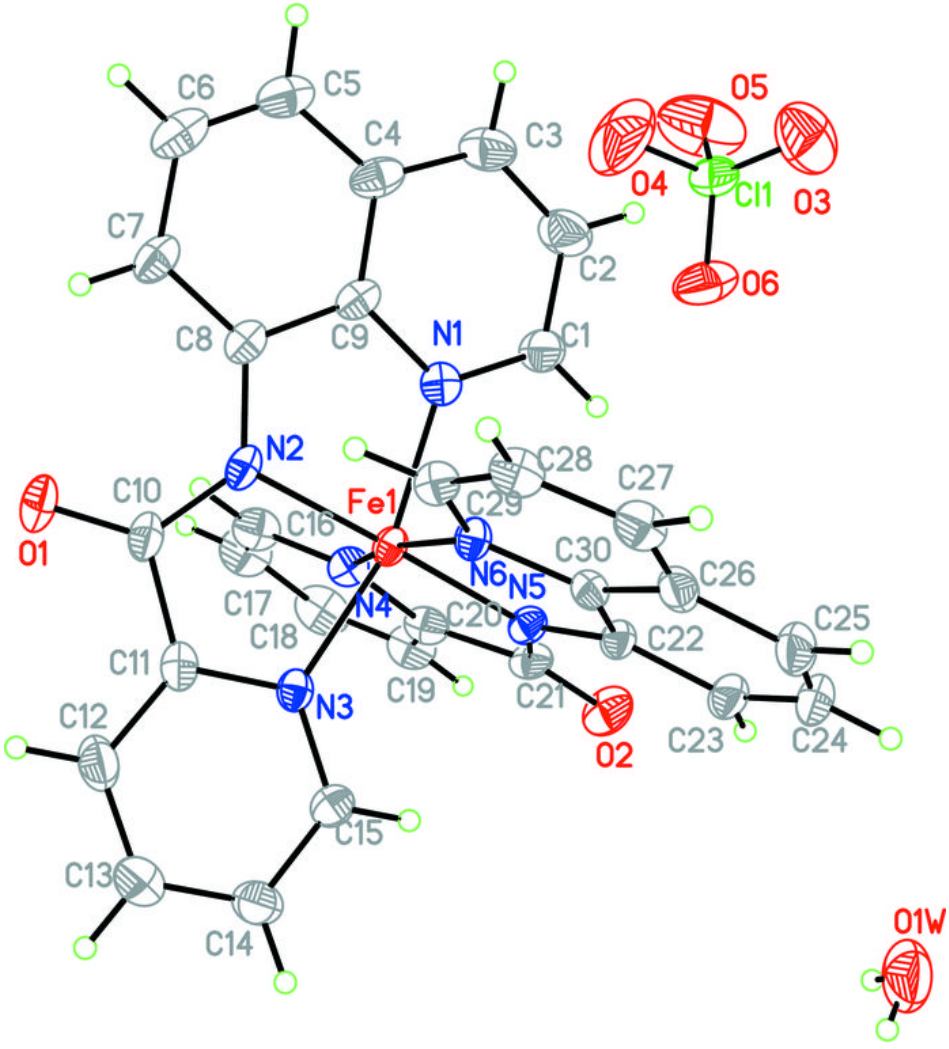
N5—C21—C20	110.7 (3)	C29—N6—Fe1	129.5 (2)
C23—C22—C30	118.8 (3)	C30—N6—Fe1	111.4 (2)
C23—C22—N5	128.1 (3)	H1W—O1W—H2W	109 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O4^{i}	0.84 (3)	2.25 (4)	2.934 (12)	139 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


C6
C5
C4
C3
O5
O4
Cl1
O3
C7
C2
O6
C8
C9
N1
C1
N2
C28
C27
C10
Fe1
C29
O1
C16
N6
N5
C30
C26
C17
N4
C20
C25
C18
C22
C11
C19
C21
N3
C12
O2
C23
C24
C15
C13
C14
O1W