Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1′-[1,4-Phenylenebis(methylene)]-dipyridinium hexacyanidoferrate(II) octahydrate

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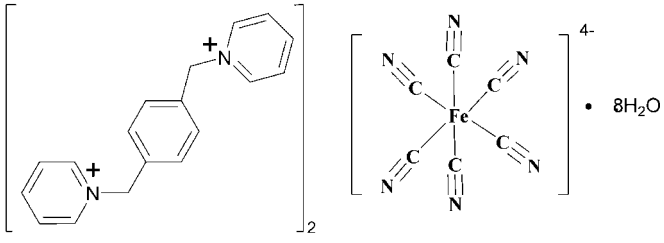
Received 25 July 2007; accepted 31 August 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.057; wR factor = 0.176; data-to-parameter ratio = 18.2.

The structure of the title complex, $(C_{18}H_{18}N_2)_2[Fe(CN)_6]\cdot 8H_2O$, comprises two 1,1′-[1,4-phenylenebis(methylene)]-dipyridinium cations, one octahedral $[Fe(CN)_6]^{4-}$ anion and eight solvent water molecules (four in the asymmetric unit); the anion and both cations are located on inversion centres. Extensive O—H···O and O—H···N hydrogen bonding involving all components of the structure leads to a three-dimensional array.

Related literature

For related literature, see: Razak *et al.* (2000); Marsh (1995); Kuchár *et al.* (2004); Overgaard *et al.* (2005); Sakai *et al.* (2004).



Experimental

Crystal data

$(C_{18}H_{18}N_2)_2[Fe(CN)_6]\cdot 8H_2O$
M_r = 880.79
Triclinic, $P\overline{1}$
a = 9.4119 (14) Å
b = 10.7164 (16) Å
c = 12.321 (3) Å
α = 104.955 (2)°
β = 101.123 (3)°
γ = 104.538 (2)°
V = 1117.2 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 291 (2) K
0.33 × 0.25 × 0.14 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.881, T_{max} = 0.946
9731 measured reflections
5049 independent reflections
3739 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.176
S = 1.00
5049 reflections
277 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H2W···N1^{i}	0.86	2.48	2.955 (5)	115
O2—H3W···N2^{ii}	0.83	2.24	2.812 (4)	127
O3—H6W···N3^{iii}	0.83	2.10	2.876 (4)	157
O4—H7W···N1^{iv}	0.83	2.21	3.029 (4)	168
O4—H8W···O3^{i}	0.83	1.91	2.729 (4)	168
O4—H8W···O3^{i}	0.83	1.91	2.729 (4)	168
O4—H7W···N1^{iv}	0.83	2.21	3.029 (4)	168
O3—H6W···N3^{iii}	0.83	2.10	2.876 (4)	157
O3—H5W···O2	0.82	1.91	2.702 (4)	161
O2—H3W···N2^{ii}	0.83	2.24	2.812 (4)	127
O1—H2W···N1^{i}	0.86	2.48	2.955 (5)	115
O1—H1W···O4	0.85	2.01	2.792 (5)	152

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y+1, z+1$; (iii) $x, y, z+1$; (iv) $x+1, y+1, z$.

Data collection: *APEX2* (Bruker, 2001); 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 the National Natural Science Foundation (No. 20671083), the Henan Province Excellent Young Foundation (No. 0612002800), and Jinan Henghua Science and Technology Co. Ltd for supporting this work. We also thank Luoyang Normal College for the diffraction measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2041).

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 doi:10.1107/S1600536807042705

supplementary materials

Acta Cryst. (2007). E**63**, m2517 [**doi:10.1107/S1600536807042705**]

1,1'-[1,4-Phenylenebis(methylene)]dipyridinium hexacyanidoferrate(II) octahydrate

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Comment

Organo-inorganic hybrid compounds containing hexacyanoferrate(II) anions have been the subject of numerous investigations, in which the cations used to balance the charges are mainly metal complex or alkyammonium (Razak *et al.*, 2000; Marsh, 1995; Kuchár *et al.*, 2004; Overgaard *et al.*, 2005; Sakai *et al.*, 2004). In this work we present the crystal structure of a novel compound with 1,1'-(1,4-phenylenebis(methylene))dipyridinium cations.

The crystal structure of the title compound, $((C_{18}H_{18}N_2)^{2+})_2[Fe(CN)_6].4\,H_2O$, has been determined by single-crystal X-ray diffraction. It consists of discrete 1,1'-(1,4-phenylenebis(methylene))dipyridinium cations and hexacyanoferrate(II) anions. The site symmetry of the cations as well as the anion is −1. The structure comprises $(C_{18}H_{18}N_2)^{2+}$ cations, $[Fe(CN)_6]^{4-}$ anions and water molecules in the ratio 2:1:8 (Figs. 1 and 2). The anions show the expected octahedral coordination with only minor deviations from the ideal geometry. By contrast, the conformations of the cations differ slightly. Extensive hydrogen bonding is found in the crystal structure involving all constituents, shown in Table 1.

Experimental

All chemicals were used as purchased from Jinan Henghua Sci. and Tec·Co., Ltd. The salt was synthesized from the reaction of 1,1'-(1,4-phenylenebis(methylene))dipyridinium dichloride (0.067 g, 0.2 mmol) in methanol (5 ml) and $K_4[Fe(CN)_6]$(0.037 g, 0.1 mmol) in DMF (10 ml). The mixture was set aside for the formation of pink crystals in 43% yield after several days. Anal. Calc. for $C_{42}H_{52}FeN_{10}O_8$: C 57.21, H 5.90, N 15.89, Fe 6.36%; Found: C 57.24, H 5.96, N 15.92, Fe 6.39%.

Refinement

All H atoms on C atoms were generated geometrically and refined as riding atoms with C—H= 0.93Å and U_{iso}(H)= 1.2 U_{eq}(C). The H atoms of the water molecule were located in a difference Fourier map.

Figures

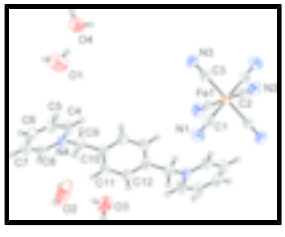

Fig. 1. The molecular structure of the title compound except the second cation, displacement ellipsoids drawn at the 50% probability level. Unlabeled atoms in the anion are related to labeled atoms by −*x*, −*y*, −*z*. Unlabeled atoms in the dication are related to labeled atoms by −*x*, 1 − *y*, 1 − *z*.

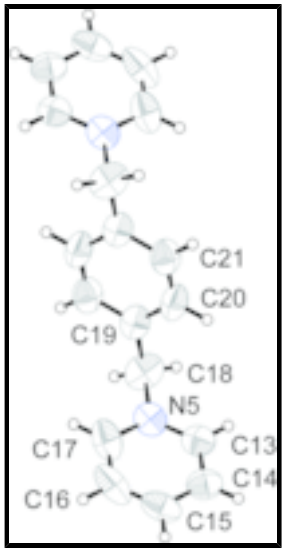

Fig. 2. The molecular structure of the second cation in the title compound, displacement ellipsoids drawn at the 50% probability level. Unlabeled atoms are related to labeled atoms by 1 − *x*, 1 − *y*, 1 − *z*.

1,1'-[1,4-Phenylenebis(methylene)]dipyridinium hexacyanidoferrate(II) octahydrate

Crystal data

$(C_{18}H_{18}N_2)_2[Fe(CN)_6]\cdot 8H_2O$	$Z = 1$
$M_r = 880.79$	$F_{000} = 464$
Triclinic, $P\overline{1}$	$D_x = 1.309$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4119$ (14) Å	Cell parameters from 2267 reflections
$b = 10.7164$ (16) Å	$\theta = 2.3$–22.2º
$c = 12.321$ (3) Å	$\mu = 0.40$ mm^{-1}
$\alpha = 104.955$ (2)º	$T = 291$ (2) K
$\beta = 101.123$ (3)º	Block, red
$\gamma = 104.538$ (2)º	0.33 × 0.25 × 0.14 mm
$V = 1117.2$ (4) Å^3	

Data collection

Bruker APEX II CCD diffractometer	5049 independent reflections
Radiation source: fine-focus sealed tube	3739 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
$T = 291(2)$ K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -12\rightarrow12$
$T_{min} = 0.881$, $T_{max} = 0.946$	$k = -13\rightarrow13$
9731 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.176$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.2979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
5049 reflections	$\Delta\rho_{max} = 0.99$ e Å^{-3}
277 parameters	$\Delta\rho_{min} = -0.37$ 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	0.0000	0.0000	0.0000	0.03288 (18)
O1	0.7215 (4)	0.9269 (4)	0.4988 (3)	0.1141 (12)
H1W	0.7419	0.8898	0.4365	0.171*
H2W	0.8049	0.9883	0.5437	0.171*
O2	0.3687 (3)	0.6379 (3)	0.9271 (4)	0.1295 (17)
H3W	0.3386	0.6919	0.8992	0.194*
H4W	0.3855	0.6601	0.9978	0.194*
O3	0.2842 (4)	0.3630 (3)	0.8512 (3)	0.1001 (11)
H5W	0.2898	0.4438	0.8649	0.150*
H6W	0.2762	0.3370	0.9080	0.150*
O4	0.8906 (3)	0.8455 (3)	0.3470 (2)	0.0822 (8)
H7W	0.9577	0.8912	0.3254	0.123*
H8W	0.8353	0.7750	0.2931	0.123*
N1	0.1041 (3)	0.0368 (3)	0.2623 (2)	0.0555 (7)
N2	0.1551 (3)	−0.2203 (3)	−0.0605 (3)	0.0539 (7)
N3	0.2958 (3)	0.2186 (2)	0.0181 (2)	0.0505 (6)
N4	0.2605 (2)	0.8518 (2)	0.6697 (2)	0.0403 (5)
N5	0.3193 (4)	0.5603 (3)	0.2302 (3)	0.0634 (8)

C1	0.0670 (3)	0.0243 (3)	0.1630 (3)	0.0394 (6)
C2	0.0958 (3)	−0.1385 (3)	−0.0374 (2)	0.0370 (6)
C3	0.1839 (3)	0.1364 (3)	0.0117 (2)	0.0368 (6)
C4	0.3744 (4)	0.8100 (3)	0.6387 (3)	0.0608 (9)
H4	0.3548	0.7458	0.5660	0.073*
C5	0.5183 (4)	0.8608 (3)	0.7125 (4)	0.0658 (10)
H5	0.5960	0.8300	0.6909	0.079*
C6	0.5478 (4)	0.9575 (3)	0.8186 (3)	0.0559 (8)
H6	0.6456	0.9934	0.8697	0.067*
C7	0.4304 (4)	1.0007 (3)	0.8485 (3)	0.0529 (7)
H7	0.4485	1.0671	0.9197	0.063*
C8	0.2873 (3)	0.9451 (3)	0.7729 (3)	0.0434 (6)
H8	0.2075	0.9729	0.7937	0.052*
C9	0.1039 (3)	0.7955 (3)	0.5867 (3)	0.0528 (8)
H9A	0.1041	0.8296	0.5210	0.063*
H9B	0.0328	0.8262	0.6258	0.063*
C10	0.0523 (3)	0.6421 (3)	0.5428 (2)	0.0409 (6)
C11	0.0583 (3)	0.5669 (3)	0.6188 (2)	0.0478 (7)
H11	0.0971	0.6112	0.6989	0.057*
C12	0.0068 (3)	0.4262 (3)	0.5759 (3)	0.0468 (7)
H12	0.0119	0.3768	0.6277	0.056*
C13	0.1762 (5)	0.4854 (4)	0.1682 (3)	0.0637 (9)
H13	0.1498	0.3909	0.1415	0.076*
C14	0.0686 (5)	0.5463 (4)	0.1439 (3)	0.0693 (10)
H14	−0.0313	0.4936	0.1020	0.083*
C15	0.1083 (6)	0.6844 (5)	0.1813 (4)	0.0768 (12)
H15	0.0363	0.7266	0.1624	0.092*
C16	0.2515 (7)	0.7601 (5)	0.2454 (5)	0.0936 (15)
H16	0.2780	0.8546	0.2723	0.112*
C17	0.3593 (5)	0.6973 (4)	0.2714 (4)	0.0854 (13)
H17	0.4582	0.7488	0.3167	0.102*
C18	0.4348 (5)	0.4928 (5)	0.2578 (4)	0.0792 (12)
H18A	0.5285	0.5380	0.2428	0.095*
H18B	0.3979	0.3988	0.2072	0.095*
C19	0.4677 (4)	0.4967 (3)	0.3827 (3)	0.0597 (9)
C20	0.3580 (4)	0.4261 (4)	0.4245 (4)	0.0694 (10)
H20	0.2614	0.3756	0.3744	0.083*
C21	0.3904 (4)	0.4300 (4)	0.5399 (4)	0.0695 (10)
H21	0.3148	0.3819	0.5660	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0296 (3)	0.0293 (3)	0.0410 (3)	0.0110 (2)	0.0117 (2)	0.0101 (2)
O1	0.113 (3)	0.149 (3)	0.092 (2)	0.054 (3)	0.034 (2)	0.041 (2)
O2	0.0580 (17)	0.0456 (15)	0.264 (5)	0.0241 (14)	0.034 (2)	0.017 (2)
O3	0.136 (3)	0.0579 (17)	0.083 (2)	0.0022 (17)	0.0086 (19)	0.0265 (15)
O4	0.098 (2)	0.0815 (19)	0.0659 (16)	0.0213 (16)	0.0246 (15)	0.0272 (14)

N1	0.0516 (15)	0.0710 (18)	0.0459 (15)	0.0230 (14)	0.0159 (12)	0.0167 (13)
N2	0.0530 (15)	0.0417 (13)	0.0740 (18)	0.0253 (12)	0.0230 (13)	0.0162 (12)
N3	0.0433 (14)	0.0393 (13)	0.0664 (17)	0.0064 (11)	0.0217 (12)	0.0146 (12)
N4	0.0338 (11)	0.0313 (11)	0.0500 (13)	0.0069 (9)	0.0106 (10)	0.0076 (10)
N5	0.071 (2)	0.0630 (18)	0.0653 (18)	0.0276 (16)	0.0330 (16)	0.0190 (15)
C1	0.0301 (13)	0.0362 (13)	0.0520 (17)	0.0126 (11)	0.0152 (12)	0.0096 (12)
C2	0.0341 (13)	0.0338 (13)	0.0419 (14)	0.0075 (11)	0.0113 (11)	0.0128 (11)
C3	0.0377 (14)	0.0330 (13)	0.0426 (14)	0.0160 (11)	0.0134 (11)	0.0103 (11)
C4	0.0478 (18)	0.0495 (18)	0.070 (2)	0.0133 (15)	0.0224 (16)	−0.0086 (16)
C5	0.0376 (16)	0.0519 (19)	0.097 (3)	0.0148 (14)	0.0224 (17)	0.0027 (18)
C6	0.0379 (16)	0.0449 (17)	0.074 (2)	0.0060 (13)	0.0036 (15)	0.0178 (16)
C7	0.0514 (18)	0.0505 (17)	0.0479 (17)	0.0148 (15)	0.0080 (14)	0.0068 (14)
C8	0.0426 (15)	0.0424 (15)	0.0481 (16)	0.0185 (12)	0.0164 (13)	0.0115 (13)
C9	0.0417 (16)	0.0412 (16)	0.0606 (19)	0.0090 (13)	−0.0005 (14)	0.0068 (14)
C10	0.0331 (13)	0.0364 (14)	0.0456 (15)	0.0064 (11)	0.0065 (11)	0.0083 (12)
C11	0.0484 (17)	0.0473 (16)	0.0341 (14)	0.0069 (13)	0.0045 (12)	0.0041 (12)
C12	0.0483 (16)	0.0457 (16)	0.0423 (15)	0.0094 (13)	0.0079 (13)	0.0164 (13)
C13	0.083 (3)	0.062 (2)	0.0497 (19)	0.029 (2)	0.0216 (18)	0.0148 (16)
C14	0.077 (3)	0.086 (3)	0.054 (2)	0.032 (2)	0.0230 (18)	0.028 (2)
C15	0.099 (3)	0.085 (3)	0.084 (3)	0.048 (3)	0.051 (3)	0.052 (2)
C16	0.119 (4)	0.055 (2)	0.132 (4)	0.031 (3)	0.065 (4)	0.046 (3)
C17	0.079 (3)	0.064 (2)	0.111 (4)	0.008 (2)	0.043 (3)	0.026 (2)
C18	0.075 (3)	0.099 (3)	0.070 (2)	0.047 (2)	0.028 (2)	0.014 (2)
C19	0.0532 (19)	0.0539 (19)	0.069 (2)	0.0274 (16)	0.0202 (17)	0.0031 (16)
C20	0.0454 (19)	0.064 (2)	0.080 (3)	0.0104 (17)	0.0081 (18)	0.0056 (19)
C21	0.0481 (19)	0.069 (2)	0.092 (3)	0.0179 (17)	0.0256 (19)	0.023 (2)

Geometric parameters (Å, °)

Fe1—C1^{i}	1.913 (3)	C7—H7	0.9300
Fe1—C1	1.913 (3)	C8—H8	0.9300
Fe1—C3^{i}	1.918 (3)	C9—C10	1.507 (4)
Fe1—C3	1.918 (3)	C9—H9A	0.9700
Fe1—C2	1.926 (3)	C9—H9B	0.9700
Fe1—C2^{i}	1.926 (3)	C10—C12^{ii}	1.384 (4)
O1—H1W	0.8495	C10—C11	1.386 (4)
O1—H2W	0.8608	C11—C12	1.382 (4)
O2—H3W	0.8253	C11—H11	0.9300
O2—H4W	0.8141	C12—C10^{ii}	1.384 (4)
O3—H5W	0.8245	C12—H12	0.9300
O3—H6W	0.8266	C13—C14	1.362 (5)
O4—H7W	0.8282	C13—H13	0.9300
O4—H8W	0.8319	C14—C15	1.360 (6)
N1—C1	1.168 (4)	C14—H14	0.9300
N2—C2	1.157 (3)	C15—C16	1.345 (7)
N3—C3	1.165 (3)	C15—H15	0.9300
N4—C8	1.332 (4)	C16—C17	1.384 (7)
N4—C4	1.344 (4)	C16—H16	0.9300

N4—C9	1.495 (4)	C17—H17	0.9300
N5—C13	1.336 (5)	C18—C19	1.497 (5)
N5—C17	1.349 (5)	C18—H18A	0.9700
N5—C18	1.484 (5)	C18—H18B	0.9700
C4—C5	1.362 (5)	C19—C21^{iii}	1.380 (5)
C4—H4	0.9300	C19—C20	1.384 (5)
C5—C6	1.370 (5)	C20—C21	1.383 (6)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.377 (4)	C21—C19^{iii}	1.380 (5)
C6—H6	0.9300	C21—H21	0.9300
C7—C8	1.366 (4)		
C1^{i}—Fe1—C1	180.0 (3)	N4—C9—H9A	109.4
C1^{i}—Fe1—C3^{i}	90.61 (11)	C10—C9—H9A	109.4
C1—Fe1—C3^{i}	89.39 (11)	N4—C9—H9B	109.4
C1^{i}—Fe1—C3	89.39 (11)	C10—C9—H9B	109.4
C1—Fe1—C3	90.61 (11)	H9A—C9—H9B	108.0
C3^{i}—Fe1—C3	180.00 (18)	C12^{ii}—C10—C11	118.8 (3)
C1^{i}—Fe1—C2	89.07 (11)	C12^{ii}—C10—C9	119.5 (3)
C1—Fe1—C2	90.93 (11)	C11—C10—C9	121.6 (3)
C3^{i}—Fe1—C2	89.95 (10)	C12—C11—C10	120.2 (3)
C3—Fe1—C2	90.05 (10)	C12—C11—H11	119.9
C1^{i}—Fe1—C2^{i}	90.93 (11)	C10—C11—H11	119.9
C1—Fe1—C2^{i}	89.07 (11)	C11—C12—C10^{ii}	120.9 (3)
C3^{i}—Fe1—C2^{i}	90.05 (10)	C11—C12—H12	119.5
C3—Fe1—C2^{i}	89.95 (10)	C10^{ii}—C12—H12	119.5
C2—Fe1—C2^{i}	180.0 (2)	N5—C13—C14	120.5 (4)
H1W—O1—H2W	106.4	N5—C13—H13	119.7
H3W—O2—H4W	113.0	C14—C13—H13	119.7
H5W—O3—H6W	112.1	C15—C14—C13	119.6 (4)
H7W—O4—H8W	111.5	C15—C14—H14	120.2
C8—N4—C4	120.3 (3)	C13—C14—H14	120.2
C8—N4—C9	119.9 (2)	C16—C15—C14	120.1 (4)
C4—N4—C9	119.7 (3)	C16—C15—H15	120.0
C13—N5—C17	120.7 (4)	C14—C15—H15	120.0
C13—N5—C18	120.1 (3)	C15—C16—C17	119.9 (4)
C17—N5—C18	119.2 (4)	C15—C16—H16	120.0
N1—C1—Fe1	178.2 (3)	C17—C16—H16	120.0
N2—C2—Fe1	178.8 (2)	N5—C17—C16	119.2 (4)
N3—C3—Fe1	179.5 (3)	N5—C17—H17	120.4
N4—C4—C5	120.8 (3)	C16—C17—H17	120.4
N4—C4—H4	119.6	N5—C18—C19	111.5 (3)
C5—C4—H4	119.6	N5—C18—H18A	109.3
C4—C5—C6	119.6 (3)	C19—C18—H18A	109.3
C4—C5—H5	120.2	N5—C18—H18B	109.3
C6—C5—H5	120.2	C19—C18—H18B	109.3
C5—C6—C7	118.9 (3)	H18A—C18—H18B	108.0

C5—C6—H6	120.5	C21^{iii}—C19—C20	117.6 (4)
C7—C6—H6	120.5	C21^{iii}—C19—C18	120.9 (4)
C8—C7—C6	119.5 (3)	C20—C19—C18	121.4 (4)
C8—C7—H7	120.2	C21—C20—C19	120.8 (3)
C6—C7—H7	120.2	C21—C20—H20	119.6
N4—C8—C7	120.8 (3)	C19—C20—H20	119.6
N4—C8—H8	119.6	C19^{iii}—C21—C20	121.6 (4)
C7—C8—H8	119.6	C19^{iii}—C21—H21	119.2
N4—C9—C10	111.1 (2)	C20—C21—H21	119.2

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H2W···N1^{iii}	0.86	2.48	2.955 (5)	115
O2—H3W···N2^{iv}	0.83	2.24	2.812 (4)	127
O3—H6W···N3^{v}	0.83	2.10	2.876 (4)	157
O4—H7W···N1^{vi}	0.83	2.21	3.029 (4)	168
O4—H8W···O3^{iii}	0.83	1.91	2.729 (4)	168
O4—H8W···O3^{iii}	0.83	1.91	2.729 (4)	168
O4—H7W···N1^{vi}	0.83	2.21	3.029 (4)	168
O3—H6W···N3^{v}	0.83	2.10	2.876 (4)	157
O3—H5W···O2	0.82	1.91	2.702 (4)	161
O2—H3W···N2^{iv}	0.83	2.24	2.812 (4)	127
O1—H2W···N1^{iii}	0.86	2.48	2.955 (5)	115
O1—H1W···O4	0.85	2.01	2.792 (5)	152

Symmetry codes: (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, *y*+1, *z*+1; (v) *x*, *y*, *z*+1; (vi) *x*+1, *y*+1, *z*.

Fig. 1

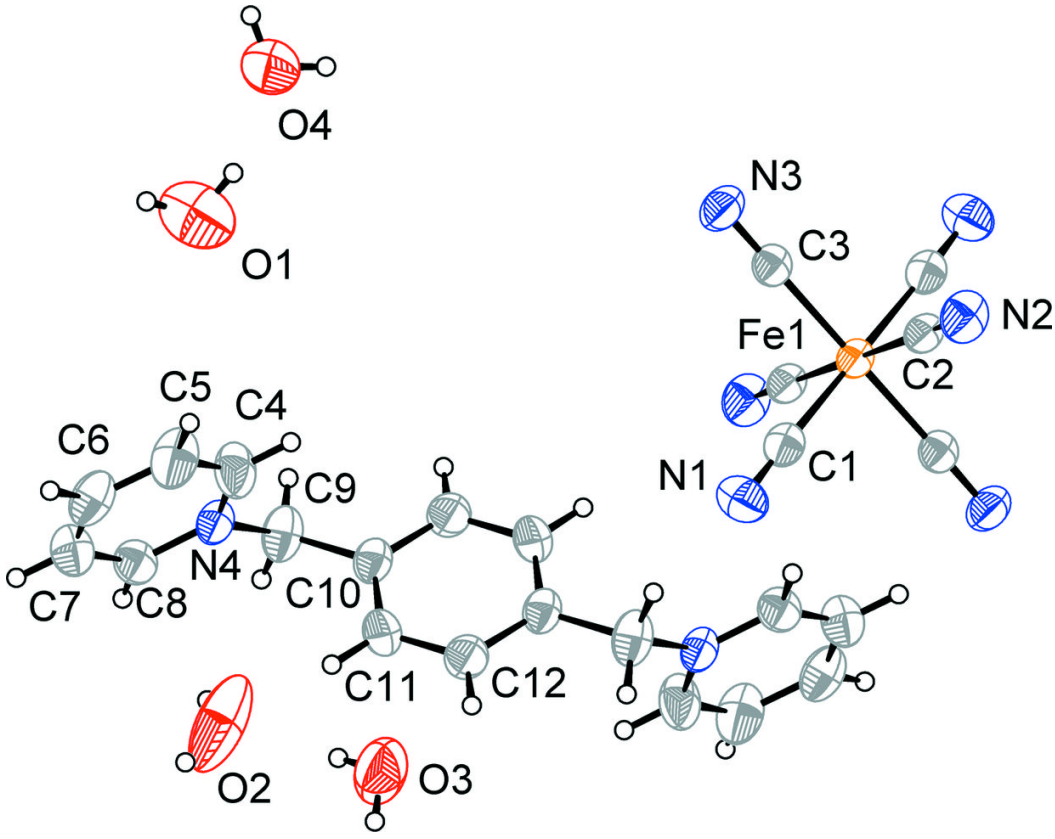

Fig. 2