Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,5:1′,5′-Bis[1,1′-(ferrocene-1,1′-diyl)-diethylidyne]dicarbonohydrazide dihydrate

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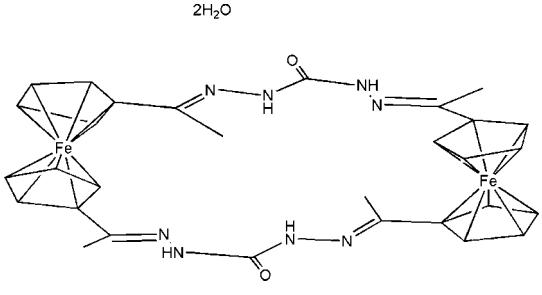
Received 11 October 2007; accepted 1 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.076; data-to-parameter ratio = 12.4.

In the title complex, $[Fe_2(C_{15}H_{16}N_4O)_2]\cdot 2H_2O$, two ferrocene units are bridged by two Schiff base linkers. This molecule lies on an inversion centre, and the asymmetric unit also contains a solvent water molecule. In the crystal structure, complexes and water molecules are connected through weak N—H···O, O—H···O, O—H···N and N—H···N hydrogen bonds.

Related literature

For related literature, see: Abuhijleh & Woods (1992); Beer (1992); Beer & Smith (1997); Li *et al.* (2006); Long (1995); Mammano *et al.* (1977); Miller & Epstein (1994); Nguyen *et al.* (1999); Seiler & Dunitz (1979); Takusagawa & Koetzle (1979).



Experimental

Crystal data

$[Fe_2(C_{15}H_{16}N_4O)_2]\cdot 2H_2O$
M_r = 684.37
Monoclinic, $C2/c$
a = 28.708 (4) Å
b = 7.9756 (11) Å
c = 15.305 (2) Å
β = 121.576 (2)°
V = 2985.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.822, T_{max} = 0.853
7443 measured reflections
2636 independent reflections
1718 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.076
S = 0.81
2636 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···N4	0.84 (3)	2.30 (3)	2.628 (3)	104 (2)
N3—H3N···O1^{i}	0.87 (3)	2.06 (3)	2.908 (3)	164 (3)
O1W—H1WA···O1	0.80 (4)	2.04 (4)	2.831 (3)	172 (4)
O1W—H1WB···N4^{ii}	0.78 (4)	2.39 (4)	3.123 (4)	156 (4)

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

Data collection: *SMART* (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: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

This work received financial support from the Natural Science Foundation of Henan Province (grant No. 0611011900) and the Foundation of Educational Department of Henan Province (grant No. 2007150012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2142).

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 doi:10.1107/S1600536807055407

supplementary materials

Acta Cryst. (2007). E**63**, m2961 [**doi:10.1107/S1600536807055407**]

1,5:1',5'-Bis[1,1'-(ferrocene-1,1'-diyl)diethylidyne]dicarbonohydrazide dihydrate

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Comment

Much attention has been paid to the chemistry of ferrocene complexes because of their potential applications in material sciences, such as molecular sensors (Beer, 1992; Beer & Smith, 1997), molecular magnetic devices (Miller & Epstein, 1994) and nonlinear optical materials (Nguyen *et al.*, 1999; Long, 1995). In continuation of our research work in the assembly and properties of ferrocene-containing Schiff base compounds (Li *et al.*, 2006), we report here the crystal structure analysis of a bis-ferrocene Schiff base compound, (I).

The compound is a cyclic bis-ferrocene complex lying on an inversion centre. The asymmetric unit is completed with a lattice water molecule. The Fe—C_{ring} bond lengths range from 2.024 (3) to 2.043 (3) Å (average: 2.034 Å) and are within the expected range (Seiler & Dunitz, 1979; Mammano *et al.*, 1977). The average intra C⋯C bond length and C⋯ C⋯C angle in cyclopentadienyl groups are 1.411 Å and 108°, which are similar to dimensions reported in the literature (Abuhijleh & Woods, 1992; Takusagawa & Koetzle, 1979). The cyclopentadienyl rings in each ferrocenyl fragment are planar and nearly parallel, with a dihedral angle of 3.7 ° at Fe1. The bond lengths N1—C11 and N4—C14 are within the normal range for C═N double bonds, while the N2—C13 and N3—C13 bond lengths suggest that they are single N—C bonds. In addition, the bond length C13═O1 is 1.216 (3) Å, consistent with a carbonyl functionality. Moreover, N1—N2 and N3—N4 bond distances are within the normal range for N—N single bonds. The two side chains are parallel by symmetry, with a torsion angle C11—C10···C4—$C14^{i}$ of about −61.6 ° [symmetry code: (i) −*x*, −*y*, −*z*].

In the crystal structure, molecules are connected by four different kinds of intra- and intermolecular hydrogen bonds. Besides the intramolecular N2—H2N···N4 and the intermolecular N3—H3N···$O1^{ii}$ interaction present in the ligand [symmetry code: (ii) −*x*, *y*, −*z* − 1/2], there are two hydrogen bonds involving the water molecule.

Experimental

All reagents were commercially available and of analytical grade. Diacetylferrocene (0.54 g, 2 mmol) and carbohydrazide (0.18 g, 2 mmol) were mixed in ethanol (15 ml). Five drops of acetic acid were added and the solution was refluxed for 4 h. Then, the solution was cooled to room temperature. Subsequently the dark-red solid formed was filtered off, washed with ethanol and dried *in vacuo* (yield: 96%). Analysis calculated for $C_{30}H_{36}Fe_2N_8O_4$: C 52.60, H 5.26, N 16.36%; found: C 52.44, H 5.24, N 16.26%.

Refinement

All H atoms bonded to C atoms were positioned geometrically and refined as riding to their carrier atoms, with C—H = 0.96–0.98 Å and U_{iso}(H) = 1.2U_{eq}(carrier C) for cyclopentadienyl and U_{iso}(H) = 1.5U_{eq}(carrier C) for methyl groups. H atoms for amine groups and water molecule were found in a difference map and refined with free coordinates and U_{iso}(H) = 1.2U_{eq}(carrier N) or U_{iso}(H) = 1.5U_{eq}(O1W).

Figures

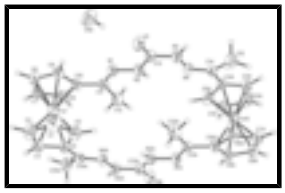


Fig. 1. The molecular structure of (I), with atom displacement ellipsoids drawn at the 50% probability level.

Bis(ferrocene-1,1'-diacetyl-carbohydrazide) dihydrate

Crystal data

$[Fe_2(C_{15}H_{16}N_4O)_2]\cdot 2H_2O$	F_{000} = 1424
M_r = 684.37	D_x = 1.523 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 398 reflections
a = 28.708 (4) Å	θ = 1.7–28.1º
b = 7.9756 (11) Å	μ = 1.02 mm^{-1}
c = 15.305 (2) Å	*T* = 293 (2) K
β = 121.576 (2)º	Irregular, red
V = 2985.5 (7) Å^3	0.20 × 0.18 × 0.16 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2636 independent reflections
Radiation source: fine-focus sealed tube	1718 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.070
T = 293(2) K	θ_{max} = 25.0º
0.3° wide ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −22→34
T_{min} = 0.822, T_{max} = 0.853	*k* = −9→9
7443 measured reflections	*l* = −18→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.076	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.81	$(\Delta/\sigma)_{max} < 0.001$

2636 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
213 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.177935 (16)	0.15125 (6)	0.29805 (3)	0.03626 (15)
N1	0.05413 (9)	0.3357 (3)	0.05970 (17)	0.0385 (6)
O1	0.03726 (8)	0.4466 (3)	−0.12140 (14)	0.0466 (6)
C1	0.21068 (14)	0.0616 (5)	0.2179 (3)	0.0588 (10)
H1A	0.2170	0.1263	0.1706	0.071*
N2	0.00660 (10)	0.3018 (3)	−0.03320 (19)	0.0403 (7)
H2N	−0.0201 (12)	0.258 (4)	−0.033 (2)	0.048*
C2	0.24803 (13)	0.0413 (5)	0.3234 (3)	0.0577 (10)
H2A	0.2848	0.0901	0.3624	0.069*
N3	−0.04608 (10)	0.3296 (3)	−0.20789 (18)	0.0414 (7)
H3N	−0.0501 (12)	0.371 (4)	−0.264 (2)	0.050*
C3	0.22351 (12)	−0.0580 (4)	0.3637 (3)	0.0498 (9)
H3A	0.2402	−0.0909	0.4357	0.060*
N4	−0.08668 (10)	0.2442 (3)	−0.20452 (18)	0.0384 (6)
C4	0.16983 (12)	−0.1025 (4)	0.2821 (2)	0.0400 (8)
C5	0.16302 (13)	−0.0266 (4)	0.1917 (2)	0.0477 (9)
H5A	0.1302	−0.0338	0.1229	0.057*
C6	0.12439 (12)	0.2452 (4)	0.3353 (2)	0.0392 (8)
H6A	0.1012	0.1788	0.3515	0.047*
C7	0.17748 (13)	0.3007 (4)	0.4061 (2)	0.0453 (9)
H7A	0.1977	0.2797	0.4801	0.054*
C8	0.19695 (13)	0.3893 (4)	0.3529 (2)	0.0473 (9)
H8A	0.2330	0.4420	0.3833	0.057*
C9	0.15578 (12)	0.3895 (4)	0.2476 (2)	0.0443 (9)
H9A	0.1582	0.4430	0.1925	0.053*
C10	0.11016 (12)	0.2996 (4)	0.2359 (2)	0.0365 (8)
C11	0.05932 (12)	0.2640 (4)	0.1388 (2)	0.0356 (7)
C12	0.01811 (12)	0.1501 (4)	0.1399 (2)	0.0523 (9)
H12A	0.0057	0.0696	0.0855	0.079*
H12B	−0.0124	0.2151	0.1303	0.079*
H12C	0.0346	0.0928	0.2045	0.079*
C13	0.00185 (13)	0.3665 (4)	−0.1192 (2)	0.0388 (8)
C14	−0.12873 (13)	0.1977 (4)	−0.2894 (2)	0.0400 (8)
C15	−0.13729 (14)	0.2308 (4)	−0.3935 (2)	0.0597 (10)
H15A	−0.1691	0.1713	−0.4445	0.090*
H15B	−0.1059	0.1935	−0.3948	0.090*
H15C	−0.1424	0.3489	−0.4077	0.090*
O1W	0.11076 (12)	0.6713 (4)	0.03268 (19)	0.0670 (8)
H1WB	0.1098 (17)	0.667 (6)	0.082 (3)	0.100*
H1WA	0.0909 (16)	0.601 (5)	−0.007 (3)	0.100*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0310 (3)	0.0420 (3)	0.0316 (3)	−0.0025 (2)	0.0135 (2)	−0.0047 (2)
N1	0.0337 (15)	0.0457 (16)	0.0271 (14)	−0.0024 (12)	0.0098 (12)	−0.0014 (13)
O1	0.0437 (14)	0.0591 (15)	0.0347 (13)	−0.0169 (12)	0.0190 (11)	−0.0079 (11)
C1	0.058 (2)	0.071 (3)	0.065 (3)	−0.013 (2)	0.044 (2)	−0.023 (2)
N2	0.0344 (17)	0.0492 (19)	0.0279 (14)	−0.0059 (12)	0.0099 (13)	0.0005 (13)
C2	0.030 (2)	0.066 (3)	0.075 (3)	−0.0046 (18)	0.027 (2)	−0.025 (2)
N3	0.0398 (16)	0.0489 (18)	0.0268 (15)	−0.0068 (14)	0.0115 (14)	0.0002 (13)
C3	0.0325 (19)	0.050 (2)	0.048 (2)	0.0086 (16)	0.0080 (17)	−0.0084 (18)
N4	0.0344 (16)	0.0410 (16)	0.0315 (15)	−0.0029 (12)	0.0115 (13)	−0.0023 (12)
C4	0.038 (2)	0.036 (2)	0.036 (2)	0.0024 (14)	0.0127 (17)	−0.0087 (14)
C5	0.046 (2)	0.056 (2)	0.040 (2)	−0.0061 (17)	0.0216 (17)	−0.0167 (17)
C6	0.040 (2)	0.047 (2)	0.0307 (18)	0.0049 (15)	0.0182 (16)	−0.0014 (15)
C7	0.049 (2)	0.047 (2)	0.0292 (18)	0.0089 (16)	0.0132 (17)	−0.0038 (15)
C8	0.041 (2)	0.044 (2)	0.041 (2)	−0.0066 (15)	0.0112 (17)	−0.0093 (16)
C9	0.042 (2)	0.044 (2)	0.0358 (19)	−0.0049 (15)	0.0128 (16)	0.0078 (15)
C10	0.038 (2)	0.041 (2)	0.0254 (17)	0.0064 (14)	0.0130 (15)	0.0015 (14)
C11	0.0341 (19)	0.0357 (18)	0.0328 (18)	0.0046 (14)	0.0146 (15)	−0.0004 (15)
C12	0.043 (2)	0.061 (2)	0.045 (2)	−0.0050 (18)	0.0174 (17)	0.0080 (18)
C13	0.043 (2)	0.037 (2)	0.0298 (18)	0.0005 (16)	0.0144 (16)	−0.0053 (15)
C14	0.039 (2)	0.0340 (19)	0.0343 (19)	0.0040 (14)	0.0104 (16)	−0.0012 (14)
C15	0.059 (2)	0.063 (3)	0.038 (2)	−0.0139 (19)	0.0119 (18)	−0.0026 (18)
O1W	0.0757 (19)	0.076 (2)	0.0496 (18)	−0.0255 (14)	0.0330 (16)	−0.0168 (15)

Geometric parameters (Å, °)

Fe1—C9	2.024 (3)	N4—C14	1.280 (3)
Fe1—C1	2.026 (3)	C4—C5	1.426 (4)
Fe1—C5	2.028 (3)	C4—C14^{i}	1.456 (4)
Fe1—C8	2.032 (3)	C5—H5A	0.9800
Fe1—C3	2.032 (3)	C6—C7	1.401 (4)
Fe1—C4	2.037 (3)	C6—C10	1.421 (4)
Fe1—C2	2.037 (3)	C6—H6A	0.9800
Fe1—C10	2.038 (3)	C7—C8	1.396 (4)
Fe1—C6	2.042 (3)	C7—H7A	0.9800
Fe1—C7	2.043 (3)	C8—C9	1.414 (4)
N1—C11	1.275 (3)	C8—H8A	0.9800
N1—N2	1.387 (3)	C9—C10	1.419 (4)
O1—C13	1.216 (3)	C9—H9A	0.9800
C1—C5	1.397 (4)	C10—C11	1.465 (4)
C1—C2	1.403 (4)	C11—C12	1.498 (4)
C1—H1A	0.9800	C12—H12A	0.9600
N2—C13	1.352 (4)	C12—H12B	0.9600
N2—H2N	0.84 (3)	C12—H12C	0.9600
C2—C3	1.399 (5)	C14—C4^{i}	1.456 (4)

C2—H2A	0.9800	C14—C15	1.503 (4)
N3—C13	1.366 (4)	C15—H15A	0.9600
N3—N4	1.374 (3)	C15—H15B	0.9600
N3—H3N	0.87 (3)	C15—H15C	0.9600
C3—C4	1.430 (4)	O1W—H1WB	0.78 (4)
C3—H3A	0.9800	O1W—H1WA	0.80 (4)
C9—Fe1—C1	104.65 (14)	C4—C3—H3A	125.8
C9—Fe1—C5	117.27 (13)	Fe1—C3—H3A	125.8
C1—Fe1—C5	40.32 (12)	C14—N4—N3	118.2 (3)
C9—Fe1—C8	40.82 (11)	C5—C4—C3	106.2 (3)
C1—Fe1—C8	118.07 (14)	C5—C4—C14^{i}	126.2 (3)
C5—Fe1—C8	152.04 (14)	C3—C4—C14^{i}	127.5 (3)
C9—Fe1—C3	162.16 (13)	C5—C4—Fe1	69.12 (18)
C1—Fe1—C3	68.09 (15)	C3—C4—Fe1	69.24 (17)
C5—Fe1—C3	68.48 (13)	C14^{i}—C4—Fe1	123.7 (2)
C8—Fe1—C3	126.80 (13)	C1—C5—C4	108.6 (3)
C9—Fe1—C4	153.31 (12)	C1—C5—Fe1	69.78 (18)
C1—Fe1—C4	68.71 (14)	C4—C5—Fe1	69.81 (17)
C5—Fe1—C4	41.07 (12)	C1—C5—H5A	125.7
C8—Fe1—C4	165.25 (12)	C4—C5—H5A	125.7
C3—Fe1—C4	41.15 (11)	Fe1—C5—H5A	125.7
C9—Fe1—C2	123.95 (15)	C7—C6—C10	108.5 (3)
C1—Fe1—C2	40.40 (13)	C7—C6—Fe1	70.02 (18)
C5—Fe1—C2	67.93 (13)	C10—C6—Fe1	69.47 (17)
C8—Fe1—C2	107.38 (14)	C7—C6—H6A	125.7
C3—Fe1—C2	40.22 (13)	C10—C6—H6A	125.7
C4—Fe1—C2	68.56 (13)	Fe1—C6—H6A	125.7
C9—Fe1—C10	40.91 (12)	C8—C7—C6	108.3 (3)
C1—Fe1—C10	123.67 (14)	C8—C7—Fe1	69.50 (18)
C5—Fe1—C10	106.42 (12)	C6—C7—Fe1	69.87 (17)
C8—Fe1—C10	68.56 (12)	C8—C7—H7A	125.8
C3—Fe1—C10	156.62 (13)	C6—C7—H7A	125.8
C4—Fe1—C10	119.98 (12)	Fe1—C7—H7A	125.8
C2—Fe1—C10	160.94 (14)	C7—C8—C9	108.3 (3)
C9—Fe1—C6	68.27 (13)	C7—C8—Fe1	70.42 (18)
C1—Fe1—C6	162.62 (13)	C9—C8—Fe1	69.30 (17)
C5—Fe1—C6	127.40 (13)	C7—C8—H8A	125.8
C8—Fe1—C6	67.67 (13)	C9—C8—H8A	125.8
C3—Fe1—C6	123.19 (14)	Fe1—C8—H8A	125.8
C4—Fe1—C6	110.05 (13)	C8—C9—C10	108.0 (3)
C2—Fe1—C6	156.61 (13)	C8—C9—Fe1	69.88 (17)
C10—Fe1—C6	40.78 (11)	C10—C9—Fe1	70.08 (17)
C9—Fe1—C7	68.12 (13)	C8—C9—H9A	126.0
C1—Fe1—C7	153.75 (14)	C10—C9—H9A	126.0
C5—Fe1—C7	165.66 (14)	Fe1—C9—H9A	126.0
C8—Fe1—C7	40.08 (12)	C9—C10—C6	106.9 (3)
C3—Fe1—C7	110.74 (13)	C9—C10—C11	126.1 (3)
C4—Fe1—C7	128.88 (13)	C6—C10—C11	127.0 (3)

C2—Fe1—C7	121.40 (13)	C9—C10—Fe1	69.02 (17)
C10—Fe1—C7	68.29 (12)	C6—C10—Fe1	69.75 (16)
C6—Fe1—C7	40.11 (11)	C11—C10—Fe1	124.1 (2)
C11—N1—N2	116.7 (3)	N1—C11—C10	115.8 (3)
C5—C1—C2	108.4 (3)	N1—C11—C12	125.6 (3)
C5—C1—Fe1	69.90 (18)	C10—C11—C12	118.7 (3)
C2—C1—Fe1	70.23 (19)	C11—C12—H12A	109.5
C5—C1—H1A	125.8	C11—C12—H12B	109.5
C2—C1—H1A	125.8	H12A—C12—H12B	109.5
Fe1—C1—H1A	125.8	C11—C12—H12C	109.5
C13—N2—N1	117.8 (3)	H12A—C12—H12C	109.5
C13—N2—H2N	122 (2)	H12B—C12—H12C	109.5
N1—N2—H2N	119 (2)	O1—C13—N2	124.6 (3)
C3—C2—C1	108.4 (3)	O1—C13—N3	120.5 (3)
C3—C2—Fe1	69.70 (18)	N2—C13—N3	114.9 (3)
C1—C2—Fe1	69.38 (19)	N4—C14—C4^{i}	116.4 (3)
C3—C2—H2A	125.8	N4—C14—C15	124.6 (3)
C1—C2—H2A	125.8	C4^{i}—C14—C15	118.9 (3)
Fe1—C2—H2A	125.8	C14—C15—H15A	109.5
C13—N3—N4	120.1 (3)	C14—C15—H15B	109.5
C13—N3—H3N	116 (2)	H15A—C15—H15B	109.5
N4—N3—H3N	123 (2)	C14—C15—H15C	109.5
C2—C3—C4	108.4 (3)	H15A—C15—H15C	109.5
C2—C3—Fe1	70.1 (2)	H15B—C15—H15C	109.5
C4—C3—Fe1	69.61 (17)	H1WB—O1W—H1WA	109 (4)
C2—C3—H3A	125.8		

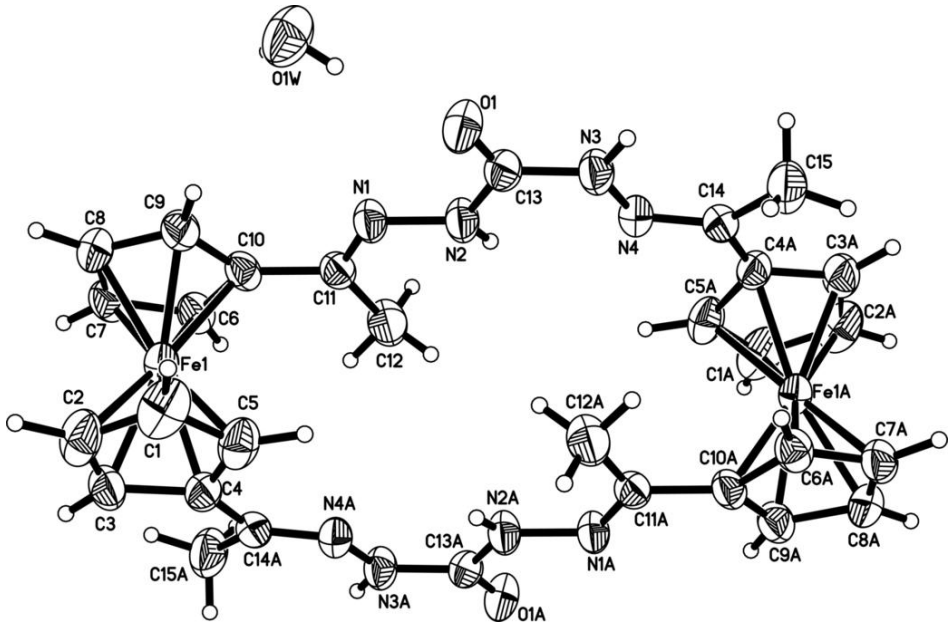
Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···N4	0.84 (3)	2.30 (3)	2.628 (3)	104 (2)
N3—H3N···O1^{ii}	0.87 (3)	2.06 (3)	2.908 (3)	164 (3)
O1W—H1WA···O1	0.80 (4)	2.04 (4)	2.831 (3)	172 (4)
O1W—H1WB···N4^{iii}	0.78 (4)	2.39 (4)	3.123 (4)	156 (4)

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

Fig. 1


O1W
O1
N3
C15
C14
N1
C13
C9
C8
C10
N2
N4
C4A
C3A
C11
C5A
C2A
C6
C7
C12
Fe1
C1A
Fe1A
C2
C5
C12A
C7A
C1
C10A
C6A
C4
N4A
N2A
C11A
C3
C13A
C8A
C14A
N1A
C9A
C15A
N3A
O1A