Electronic supplementary information

1D iron(II)-1,2,4-triazolic chains with spin crossover assembled from discrete trinuclear complexes

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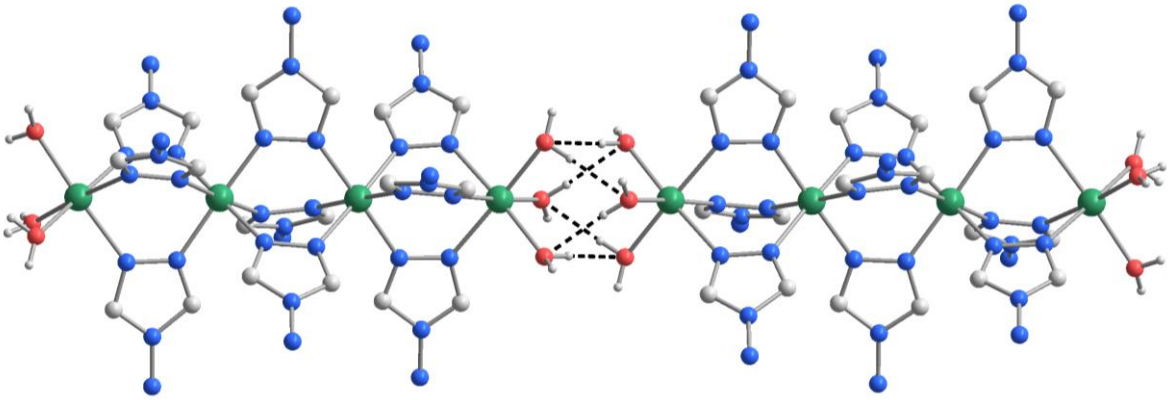
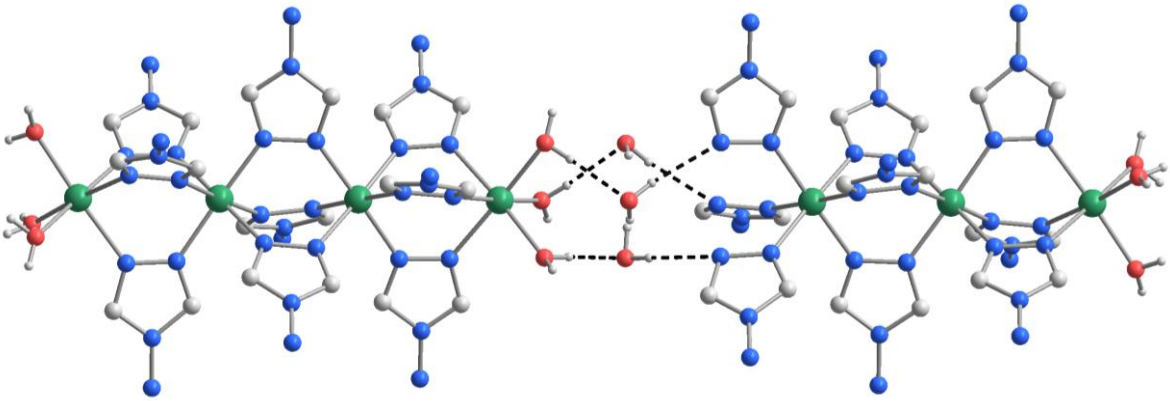
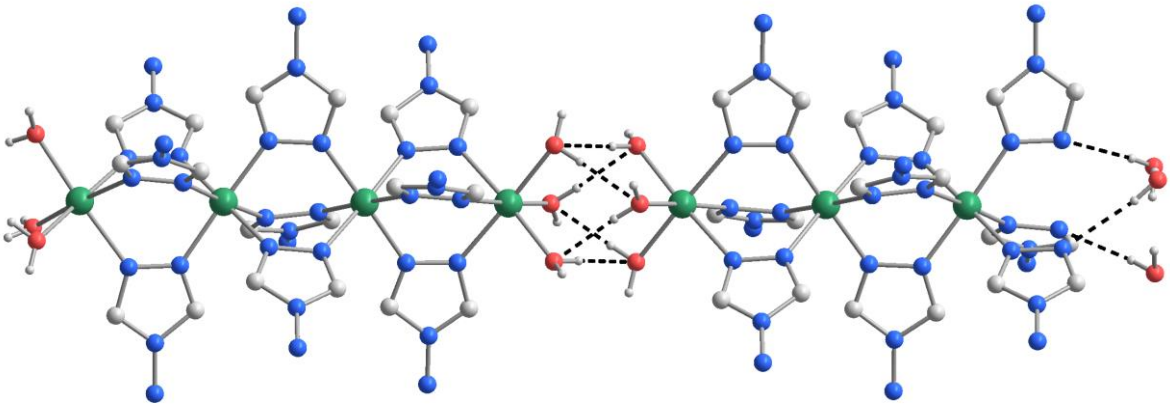
Figure S1. Possible contacts between the discrete complexes based on their nuclearity. Colour code: Fe, green; N, blue; O, red; C, gray; H, light-gray. Non-O H atoms are not shown. Selected hydrogen bonds are shown as dashed lines.

[Fe4] – [Fe4]:

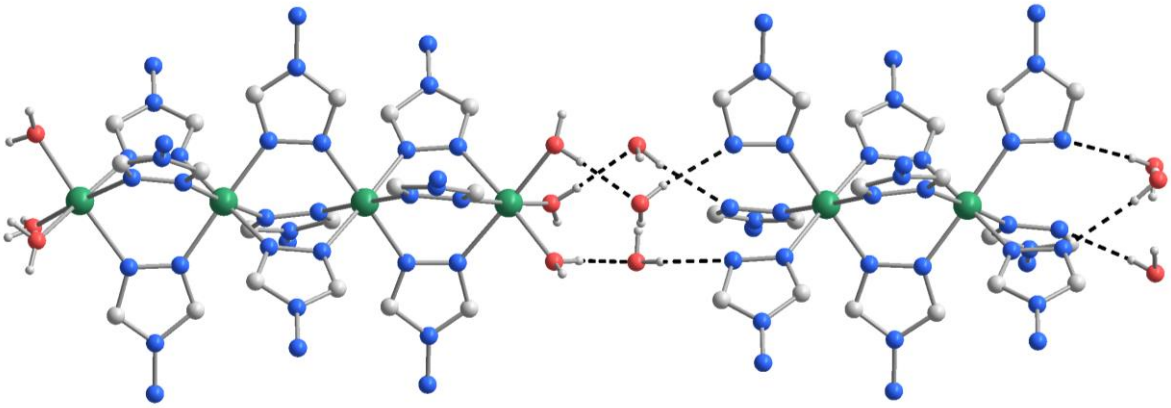


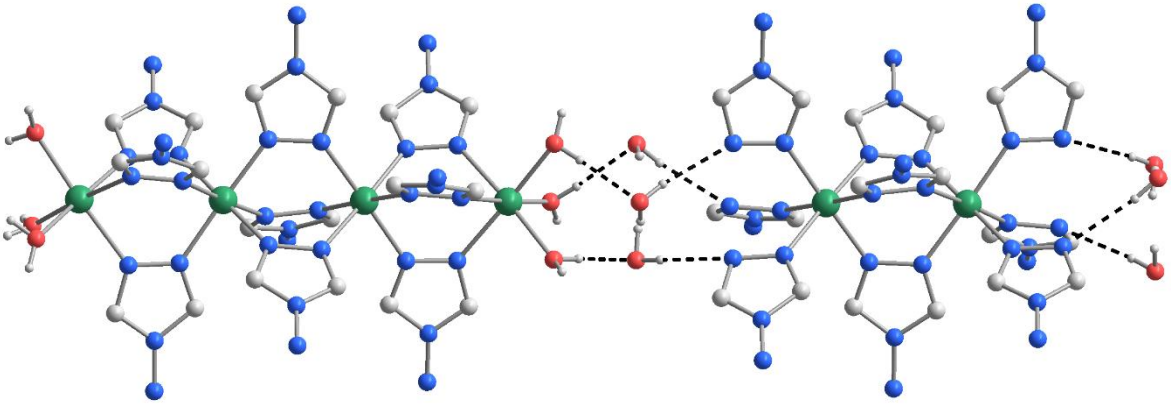
[Fe4] – [Fe3]:



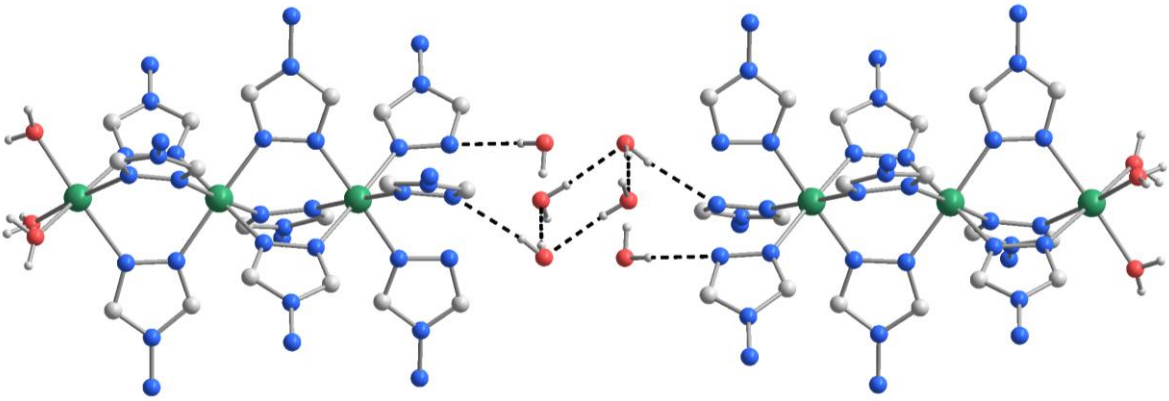


[Fe4] – [Fe2]:





[Fe3] – [Fe3]:



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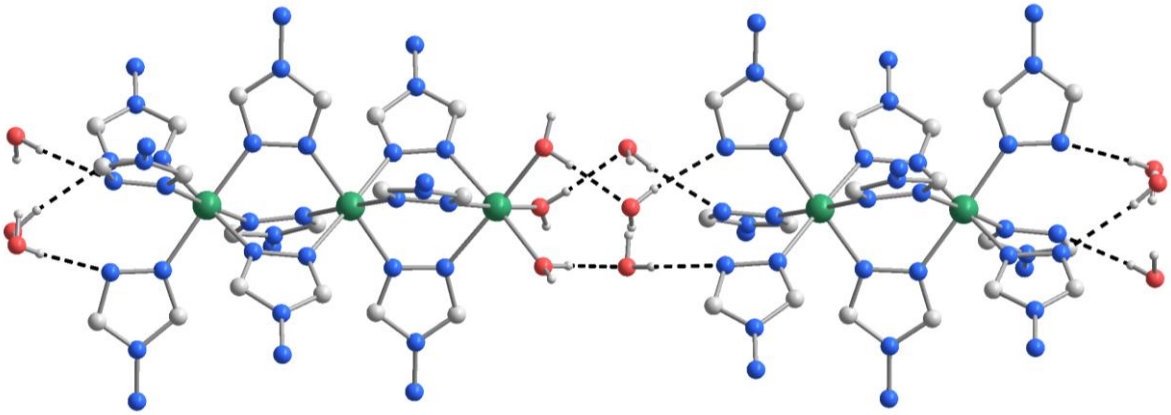
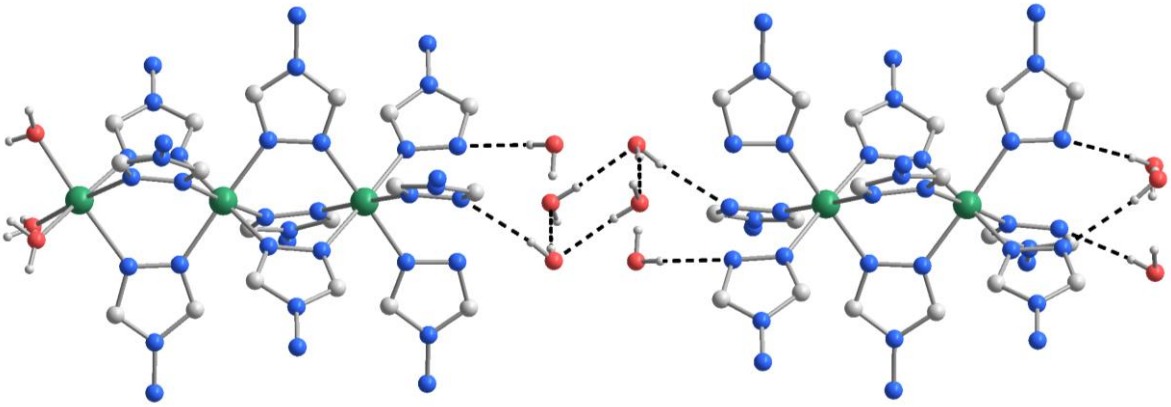
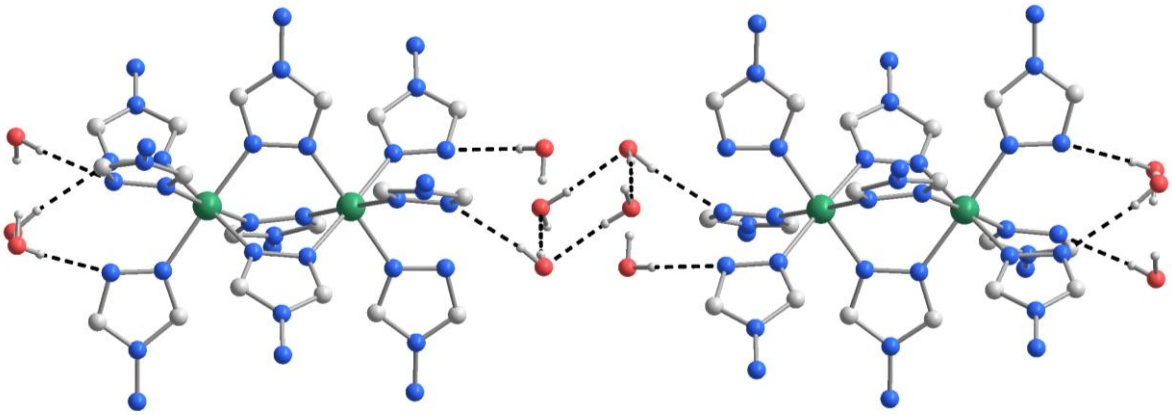




[Fe2] – [Fe2]:



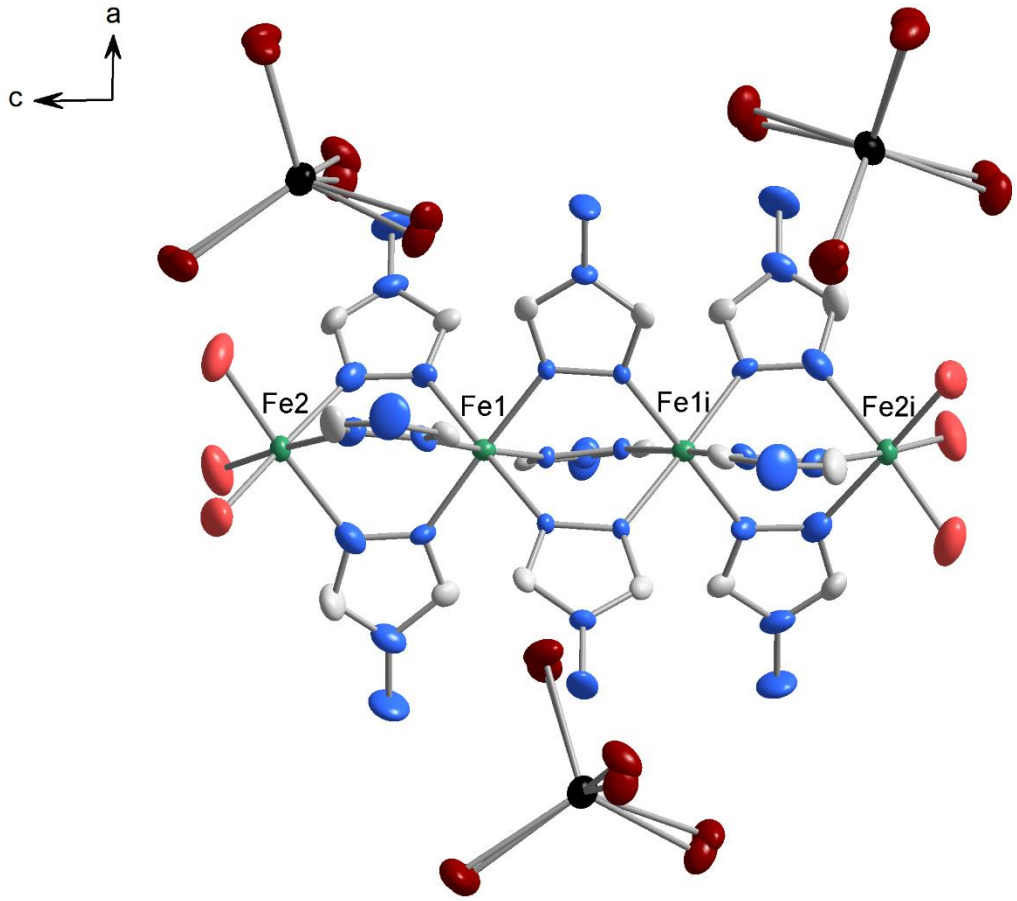


Figure S2. Fragment of the crystal structure of **1** with atomic displacement parameters drawn at 50% probability showing the molecular unit. The occupancies of Fe2 and all I atoms are 0.5. The occupancies of all other atoms are full. Colour code: Fe, green; N, blue; O, red; C, gray; Hg, black; I, brown.

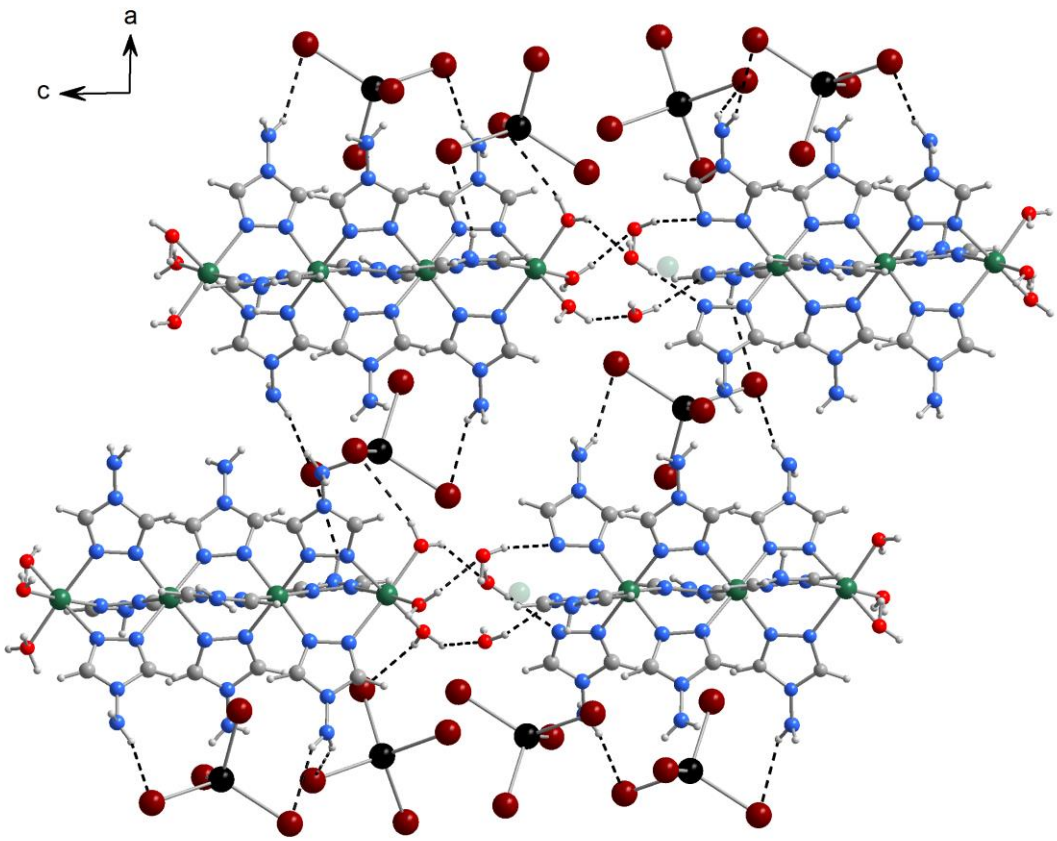


Figure S3. Crystal structure of **1** showing hydrogen bonds O–H···O, O–H···N and weak contacts N–H···I as black dashed lines. Colour code: Fe, green; N, blue; O, red; C, gray; H, light-gray; Hg, black; I, brown.

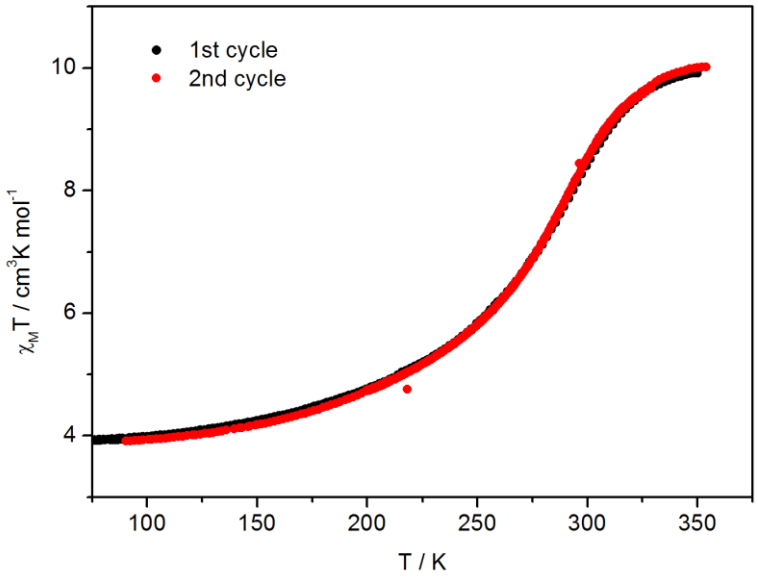


Figure S4. SCO curve of **1** recorded in two subsequent cycles of cooling and heating.

*Crystal data for **1***

$3(HgI_4)\cdot 1(C_{18}H_{48}Fe_3N_{36}O_6)$	D_x = 3.121 Mg m^{-3}
M_r = 3156.98	Mo *K*a radiation, l = 0.71073 Å
Trigonal, $R\bar{3}c$	Cell parameters from 3424 reflections
a = 19.2123 (15) Å	q = 2.8–25.0°
c = 31.531 (3) Å	m = 13.04 mm^{-1}
V = 10079.3 (18) Å^3	*T* = 173 K
Z = 6.0	Block, pink
F(000) = 8460	0.09 × 0.07 × 0.05 mm

Data collection

Bruker SMART diffractometer	R_{int} = 0.082
Absorption correction: multi-scan c.f. r.h. blessing, acta cryst. (1995), a51, 33-38	q_{max} = 26.4°, q_{min} = 1.8°
T_{min} = 0.452, T_{max} = 0.599	*h* = -24 – 12
20510 measured reflections	*k* = -11 – 23
2313 independent reflections	*l* = -39 – 39
1799 reflections with *I* > 2s(*I*)	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2s(F^2)]$ = 0.067	H-atom parameters constrained
$wR(F^2)$ = 0.158	$w = 1/[s^2(F_o^2) + (0.0314P)^2 + 1070.9049P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.22	$(D/s)_{max} < 0.001$
2313 reflections	$D\rho_{max}$ = 2.35 e Å^{-3}
139 parameters	$D\rho_{min}$ = -1.36 e Å^{-3}
0 restraints	

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

	x	***y***	***z***	U_{iso}*/U_{eq}	**Occ. (<1)**
Hg1	0.29329 (5)	0.333333	0.583333	0.0395 (3)	
I2A	0.2000 (8)	0.2857 (8)	0.5094 (4)	0.047 (2)	0.5
Fe1	0.333333	0.666667	0.47523 (11)	0.0212 (7)	
Fe2	0.333333	0.666667	0.5946 (2)	0.0255 (16)	0.5
N5	0.3383 (7)	0.5832 (7)	0.4387 (3)	0.022 (2)	
N2	0.4312 (10)	0.6825 (10)	0.5533 (5)	0.051 (4)	
N6	0.333333	0.4745 (9)	0.416667	0.030 (4)	
N3	0.5408 (10)	0.6887 (10)	0.5306 (6)	0.050 (4)	
N1	0.4265 (8)	0.6757 (8)	0.5107 (4)	0.033 (3)	
N7	0.333333	0.4010 (11)	0.416667	0.060 (7)	
H7	0.310870	0.366087	0.398570	0.071*	
C3	0.3411 (9)	0.5195 (10)	0.4508 (5)	0.029 (3)	
H3	0.347710	0.507181	0.479142	0.035*	
C1	0.4913 (10)	0.6783 (10)	0.4974 (6)	0.037 (4)	
H1	0.502783	0.673650	0.468551	0.044*	
O1	0.2341 (12)	0.6456 (12)	0.6318 (5)	0.094 (6)	
H1AA	0.231416	0.671165	0.652796	0.141*	0.5
H1AB	0.187536	0.624765	0.621316	0.141*	0.5
H1BC	0.248166	0.674845	0.609526	0.141*	0.5
H1BD	0.257286	0.617155	0.634146	0.141*	0.5
C2	0.5016 (14)	0.6887 (14)	0.5636 (6)	0.055 (6)	
H2	0.520392	0.692756	0.591827	0.066*	
N4	0.6142 (11)	0.6938 (14)	0.5302 (7)	0.079 (6)	
H4A	0.643674	0.683409	0.514774	0.095*	
H4B	0.644834	0.742779	0.534914	0.095*	
I1A	0.4346 (6)	0.4710 (6)	0.5607 (3)	0.0453 (15)	0.5
I2B	0.1956 (8)	0.3019 (7)	0.5139 (4)	0.048 (2)	0.5
I1B	0.4484 (6)	0.4578 (7)	0.5600 (4)	0.0495 (19)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0426 (6)	0.0412 (4)	0.0351 (5)	0.0213 (3)	-0.0076 (4)	-0.0038 (2)
I2A	0.069 (5)	0.043 (4)	0.040 (2)	0.035 (3)	0.009 (2)	-0.002 (2)
Fe1	0.0196 (10)	0.0196 (10)	0.0245 (17)	0.0098 (5)	0.000	0.000
Fe2	0.029 (2)	0.029 (2)	0.019 (3)	0.0144 (12)	0.000	0.000
N5	0.025 (6)	0.022 (6)	0.017 (6)	0.012 (5)	0.002 (5)	0.001 (5)
N2	0.055 (10)	0.046 (10)	0.052 (10)	0.026 (8)	-0.019 (8)	-0.008 (8)
N6	0.032 (10)	0.023 (7)	0.038 (11)	0.016 (5)	0.002 (8)	0.001 (4)
N3	0.048 (10)	0.045 (9)	0.068 (11)	0.031 (8)	-0.017 (9)	-0.004 (8)
N1	0.024 (7)	0.037 (8)	0.037 (8)	0.015 (6)	0.009 (6)	0.011 (6)
N7	0.10 (2)	0.041 (9)	0.055 (15)	0.051 (11)	0.013 (14)	0.006 (7)
C3	0.018 (7)	0.035 (9)	0.030 (8)	0.010 (7)	0.007 (6)	0.008 (7)
C1	0.036 (10)	0.034 (9)	0.042 (10)	0.019 (8)	0.005 (8)	0.013 (8)
O1	0.127 (17)	0.136 (18)	0.056 (10)	0.091 (15)	0.028 (11)	0.027 (11)
C2	0.075 (15)	0.074 (15)	0.037 (11)	0.053 (13)	-0.009 (11)	0.006 (10)
N4	0.056 (12)	0.117 (18)	0.091 (15)	0.064 (13)	-0.017 (11)	-0.006 (14)
I1A	0.034 (3)	0.064 (4)	0.047 (3)	0.031 (3)	-0.001 (2)	-0.005 (3)
I2B	0.056 (4)	0.061 (6)	0.041 (4)	0.039 (4)	-0.011 (3)	-0.015 (3)
I1B	0.045 (4)	0.057 (4)	0.059 (3)	0.035 (4)	0.013 (3)	0.022 (4)

Geometric parameters (Å, º)

Hg1—I2A^{i}	2.801 (14)	N5—C3	1.310 (19)
Hg1—I2A	2.802 (15)	N2—N1	1.35 (2)
Hg1—I1A^{i}	2.774 (10)	N2—C2	1.34 (3)
Hg1—I1A	2.774 (11)	N6—N7	1.41 (3)
Hg1—I2B	2.747 (14)	N6—C3^{iv}	1.340 (19)
Hg1—I2B^{i}	2.746 (14)	N6—C3	1.340 (19)
Hg1—I1B	2.831 (12)	N3—C1	1.36 (2)
Hg1—I1B^{i}	2.831 (11)	N3—C2	1.29 (3)
Fe1—N5^{ii}	2.015 (12)	N3—N4	1.36 (2)
Fe1—N5^{iii}	2.015 (12)	N1—C1	1.29 (2)

Fe1—N5	2.015 (11)	N7—H7^{iv}	0.8202
Fe1—N1^{iii}	2.043 (14)	N7—H7	0.8201
Fe1—N1^{ii}	2.043 (14)	C3—H3	0.9500
Fe1—N1	2.043 (14)	C1—H1	0.9500
Fe2—N2^{ii}	2.178 (19)	O1—H1AA	0.8406
Fe2—N2^{iii}	2.178 (18)	O1—H1AB	0.8434
Fe2—N2	2.178 (18)	O1—H1BC	0.8554
Fe2—O1^{iii}	2.100 (18)	O1—H1BD	0.8638
Fe2—O1	2.100 (18)	C2—H2	0.9500
Fe2—O1^{ii}	2.100 (18)	N4—H4A	0.8427
N5—N5^{iv}	1.40 (2)	N4—H4B	0.8368
I2A—Hg1—I2A^{i}	123.1 (4)	O1^{iii}—Fe2—N2^{iii}	176.4 (7)
I2A^{i}—Hg1—I1B^{i}	106.9 (4)	O1—Fe2—N2^{ii}	88.4 (7)
I2A—Hg1—I1B^{i}	108.1 (3)	O1^{ii}—Fe2—N2	91.8 (6)
I1A^{i}—Hg1—I1A	119.8 (3)	O1^{ii}—Fe2—O1^{iii}	91.7 (7)
I1A^{i}—Hg1—I1B^{i}	9.2 (2)	O1—Fe2—O1^{iii}	91.7 (7)
I1A^{i}—Hg1—I1B	110.78 (14)	O1—Fe2—O1^{ii}	91.7 (7)
I1A—Hg1—I1B	9.2 (2)	N5^{iv}—N5—Fe1	124.3 (4)
I1A—Hg1—I1B^{i}	110.78 (14)	C3—N5—Fe1	128.1 (10)
I2B—Hg1—I1A	103.9 (3)	C3—N5—N5^{iv}	107.1 (9)
I2B^{i}—Hg1—I1A	109.6 (3)	N1—N2—Fe2	124.8 (12)
I2B^{i}—Hg1—I2B	110.0 (4)	C2—N2—Fe2	129.2 (14)
I2B—Hg1—I1B^{i}	115.4 (3)	C2—N2—N1	105.3 (16)
I2B—Hg1—I1B	107.1 (3)	C3^{iv}—N6—N7	126.1 (9)
I2B^{i}—Hg1—I1B	115.4 (3)	C3—N6—N7	126.1 (9)
I2B^{i}—Hg1—I1B^{i}	107.1 (3)	C3—N6—C3^{iv}	107.8 (19)
I1B—Hg1—I1B^{i}	101.9 (3)	C1—N3—N4	128.8 (18)
N5^{ii}—Fe1—N5^{iii}	90.5 (5)	C2—N3—C1	104.8 (16)
N5^{ii}—Fe1—N5	90.5 (5)	C2—N3—N4	126.2 (18)
N5^{iii}—Fe1—N5	90.5 (5)	N2—N1—Fe1	124.5 (11)
N5^{ii}—Fe1—N1^{iii}	87.0 (5)	C1—N1—Fe1	127.8 (12)
N5^{iii}—Fe1—N1^{ii}	177.5 (5)	C1—N1—N2	107.7 (15)
N5—Fe1—N1	89.6 (5)	N6—N7—H7^{iv}	123.712 (8)
N5^{iii}—Fe1—N1	87.0 (5)	N6—N7—H7	123.7
N5^{iii}—Fe1—N1^{iii}	89.6 (5)	H7—N7—H7^{iv}	112.6
N5^{ii}—Fe1—N1^{ii}	89.6 (5)	N5—C3—N6	109.0 (14)
N5—Fe1—N1^{ii}	87.0 (5)	N5—C3—H3	125.5

N5^{ii}—Fe1—N1	177.5 (5)	N6—C3—H3	125.5
N5—Fe1—N1^{iii}	177.5 (5)	N3—C1—H1	124.9
N1^{iii}—Fe1—N1	92.9 (5)	N1—C1—N3	110.2 (16)
N1^{ii}—Fe1—N1	92.9 (5)	N1—C1—H1	124.9
N1^{iii}—Fe1—N1^{ii}	92.9 (5)	Fe2—O1—H1AA	129.9
N2^{iii}—Fe2—N2	88.0 (6)	Fe2—O1—H1AB	121.1
N2^{ii}—Fe2—N2	88.0 (6)	H1AA—O1—H1AB	103.1
N2^{iii}—Fe2—N2^{ii}	88.0 (6)	H1BC—O1—H1BD	113.0
O1^{ii}—Fe2—N2^{iii}	88.4 (7)	N2—C2—H2	124.1
O1—Fe2—N2^{iii}	91.8 (6)	N3—C2—N2	111.8 (18)
O1^{ii}—Fe2—N2^{ii}	176.4 (7)	N3—C2—H2	124.1
O1^{iii}—Fe2—N2	88.4 (7)	N3—N4—H4A	141.2
O1^{iii}—Fe2—N2^{ii}	91.8 (6)	N3—N4—H4B	101.5
O1—Fe2—N2	176.4 (7)	H4A—N4—H4B	101.0
Fe1—N5—C3—N6	172.1 (8)	N7—N6—C3—N5	−179.9 (7)
Fe1—N1—C1—N3	176.8 (11)	C3^{iv}—N6—C3—N5	0.1 (7)
Fe2—N2—N1—Fe1	10 (2)	C1—N3—C2—N2	−3 (2)
Fe2—N2—N1—C1	−171.7 (12)	C2—N2—N1—Fe1	−178.5 (13)
Fe2—N2—C2—N3	172.8 (13)	C2—N2—N1—C1	0 (2)
N5^{iv}—N5—C3—N6	−0.2 (18)	C2—N3—C1—N1	2 (2)
N2—N1—C1—N3	−1.4 (19)	N4—N3—C1—N1	179.4 (19)
N1—N2—C2—N3	2 (2)	N4—N3—C2—N2	−179.7 (19)

Symmetry codes: (i) x−y+1/3, −y+2/3, −z+7/6; (ii) −x+y, −x+1, z; (iii) −y+1, x−y+1, z; (iv) −x+2/3, −x+y+1/3, −z+5/6.