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Bis(μ-3,5-di-2-pyridyl-1,2,4-triazolato-$\kappa^4N^1,N^5:N^2,N^3$)bis[(methanol-κO)(thiocyanato-κN)iron(II)]

Gang-Biao Jiang,[a] Xin-Nian Zeng,[a] Yu-Sheng Fang,[a] Ming-Hua Zeng[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Guangxi Normal University, Guilin 541000, Guangxi, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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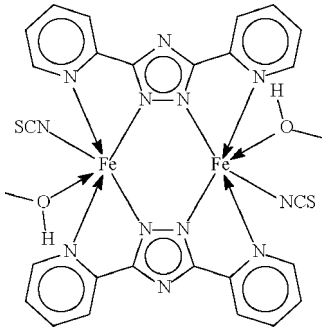
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.091; data-to-parameter ratio = 15.5.

In the title centrosymmetric dinuclear iron(II) compound, $[Fe_2(C_{12}H_8N_5)_2(NCS)_2(CH_4O)_2]$, the deprotonated 3,5-di-2-pyridyl-1,2,4-triazole ligand uses a pair of $N_{pyridyl}/N_{triazolyl}$ atoms to chelate one metal atom and the other pair of $N_{pyridyl}/N_{triazolyl}$ atoms to chelate the other metal atom. Each Fe atom is octahedrally coordinated by four N atoms surrounding the metal center in a square-planar environment. Above and below this plane are located the N atom of the thiocyanate anion and the O atom of the methanol molecule. Intermolecular O—H···N hydrogen bonding gives rise to a layer motif.

Related literature

For a review of the coordination chemistry of 3,5-di-2-pyridyl-1,2,4-triazoles and related *N*-heterocycles, see Klingele & Brooker (2003). For the crystal structures of dinuclear derivatives of the deprotonated ligand, see Chen, Hu *et al.* (2006) and Chen, Zhou *et al.* (2006).



Experimental

Crystal data

$[Fe_2(C_{12}H_8N_5)_2(NCS)_2(CH_4O)_2]$
M_r = 736.41
Monoclinic, $P2_1/c$
a = 11.5051 (8) Å
b = 14.291 (1) Å
c = 9.7794 (7) Å
β = 102.885 (1)°
V = 1567.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 295 (2) K
0.35 × 0.20 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.698, T_{max} = 0.826
8319 measured reflections
3302 independent reflections
2827 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.092
S = 1.02
3302 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N4^{i}	0.82 (3)	1.89 (3)	2.698 (2)	169 (3)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2467).

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supplementary materials

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Bis(μ-3,5-di-2-pyridyl-1,2,4-triazolato-$\kappa^4N^1,N^5:N^2,N^3$)bis[(methanol-κO)(thiocyanato-κN)iron(II)]

G.-B. Jiang, X.-N. Zeng, Y.-S. Fang, M.-H. Zeng and S. W. Ng

Comment

The coordination chemistry of the class of 3,5-di-2-pyridyl-1,2,4-triazole *N*-heterocycles has been reviewed (Klingele & Brooker, 2003). The deprotonated 3,5-di-2-pyridyl-1,2,4-triazole monoanion is capable of using the pyridyl as well as the triazolyl nitrogen atoms to coordinate to more than one metal center, as noted in the trichloridodicopper(I)copper(II) (Chen, Zhou *et al.*, 2006) and tetrachloridodiiron(III) and dichloridodiiron(II) (Chen, Hu *et al.*, 2006) complexes. Centrosymmetric dinuclear $(C_{12}H_8N_5)_2(CH_4O)_2(NCS)_2Fe_2$ has the deprotonated ligand using a pair of $N'_{pyridyl}/N^1$ atoms to chelate to one metal atom and its other pair of $N''_{pyridyl}/N^2$ atoms to chelate to the other metal atom, the four nitrogen atoms approximating a square. The six-coordinate environment has the nitrogen atom of the thiocyanate anion and the oxygen atom of the methanol molecule in the other two sites of the octahedron. Intermolecular hydrogen bonding between the hydroxy group and the 4-nitrogen atom of the ligand gives rise to a layer motif.

Experimental

4-Amino-3,5-di-2-pyridyl-1,2,4-triazole was purchased from Aldrich Chemical Company. 3,5-di-2-pyridyl-1,2,4-triazole was synthesized by the deammoniation of the compound. Sulfuric acid (2*M*, 20 ml) was added to a mixture of the compound (11.9 g, 0.05 mol) and sodium nitrite (3.45 g, 0.05 mol) at 273 K. Hypophosphorus acid (0.05 mol) when added gave an immediate precipitate, which was then purified by recrystallization from ethanol (80% yield). 3,5-di-2-pyridyl-1,2,4-triazole, ferrous sulfate and potassium thiocyanate (0.1 mmol each) were suspended in methanol (8 ml). The suspension was heated in a 23-ml, Teflon-lined Parr bomb at 383 K for 96 h. The bomb was then cooled at 5 K h^{-1} to room temperature. Block-shaped crystals were picked by hand (40% yield).

Refinement

Carbon-bound H atoms were placed at calculated positions (C–H 0.93 – 0.96 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 – 1.5 times U_{eq}(C). The hydroxy H atom was located in a difference Fourier map, and its positional and displacement parameters were refined.

Figures

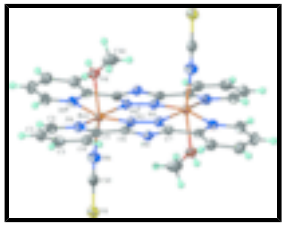

Fig. 1. Thermal ellipsoid plot of $(C_{12}H_8N_5)_2(CH_4O)_2(NCS)_2Fe_2$. Displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radii.

Bis[μ-3,5-di-2-pyridyl-1,2,4-triazolato-\ κ$^4N^1$,N^5:N^2,N^3]bis[(methanol-\ κO)(thiocyanato-κN)iron(II)]

Crystal data

$[Fe_2(C_{12}H_8N_5)_2(NCS)_2(CH_4O)_2]$	F_{000} = 752
M_r = 736.41	D_x = 1.560 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3100 reflections
a = 11.5051 (8) Å	θ = 2.3–27.0º
b = 14.291 (1) Å	μ = 1.11 mm^{-1}
c = 9.7794 (7) Å	T = 295 (2) K
β = 102.885 (1)º	Block, black
V = 1567.4 (2) Å^3	0.35 × 0.20 × 0.18 mm
Z = 2	

Data collection

Bruker APEX area-detector diffractometer	3302 independent reflections
Radiation source: fine-focus sealed tube	2827 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 293(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −14→13
T_{min} = 0.698, T_{max} = 0.826	k = −17→18
8319 measured reflections	l = −9→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.092	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3302 reflections	$\Delta\rho_{max}$ = 0.75 e Å^{-3}
213 parameters	$\Delta\rho_{min}$ = −0.27 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	0.64986 (2)	0.524340 (19)	0.41164 (3)	0.01615 (11)
S1	0.95226 (5)	0.42521 (5)	0.81308 (6)	0.02961 (16)
O1	0.54102 (13)	0.57952 (11)	0.21963 (16)	0.0211 (3)
H1o	0.541 (2)	0.636 (2)	0.207 (3)	0.038 (8)*
N1	0.70485 (15)	0.41319 (12)	0.26974 (19)	0.0207 (4)
N2	0.53238 (15)	0.40957 (12)	0.40463 (18)	0.0178 (4)
N3	0.44253 (14)	0.39173 (11)	0.47076 (18)	0.0175 (4)
N4	0.47467 (15)	0.26108 (11)	0.35794 (18)	0.0178 (4)
N5	0.26895 (15)	0.32792 (12)	0.58072 (18)	0.0199 (4)
N6	0.78557 (18)	0.48169 (13)	0.5746 (2)	0.0271 (4)
C1	0.79195 (19)	0.42006 (16)	0.2001 (2)	0.0253 (5)
H1	0.8348	0.4757	0.2064	0.030*
C2	0.82160 (19)	0.34804 (17)	0.1186 (2)	0.0264 (5)
H2	0.8822	0.3559	0.0706	0.032*
C3	0.7597 (2)	0.26473 (16)	0.1102 (2)	0.0251 (5)
H3	0.7786	0.2152	0.0573	0.030*
C4	0.66880 (18)	0.25605 (14)	0.1818 (2)	0.0214 (5)
H4	0.6258	0.2006	0.1778	0.026*
C5	0.64317 (18)	0.33118 (14)	0.2593 (2)	0.0192 (4)
C6	0.54899 (17)	0.33112 (14)	0.3386 (2)	0.0165 (4)
C7	0.41065 (17)	0.30331 (14)	0.4418 (2)	0.0166 (4)
C8	0.31801 (17)	0.26428 (14)	0.5074 (2)	0.0185 (4)
C9	0.28571 (18)	0.17074 (15)	0.4987 (2)	0.0224 (5)
H9	0.3199	0.1291	0.4459	0.027*
C10	0.20137 (19)	0.14047 (17)	0.5702 (2)	0.0256 (5)
H10	0.1795	0.0777	0.5680	0.031*
C11	0.1505 (2)	0.20409 (17)	0.6443 (2)	0.0274 (5)
H11	0.0937	0.1852	0.6928	0.033*
C12	0.18556 (18)	0.29756 (16)	0.6456 (2)	0.0247 (5)
H12	0.1492	0.3407	0.6937	0.030*
C13	0.85569 (19)	0.45901 (15)	0.6734 (2)	0.0221 (5)
C14	0.4317 (2)	0.53995 (17)	0.1449 (3)	0.0333 (6)
H14A	0.4008	0.5766	0.0626	0.050*
H14B	0.3752	0.5395	0.2039	0.050*
H14C	0.4453	0.4770	0.1179	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01877 (17)	0.01035 (18)	0.01979 (18)	−0.00042 (11)	0.00532 (12)	−0.00032 (11)
S1	0.0239 (3)	0.0385 (4)	0.0252 (3)	0.0026 (3)	0.0028 (2)	0.0052 (3)
O1	0.0241 (8)	0.0122 (8)	0.0251 (8)	−0.0013 (6)	0.0019 (6)	0.0026 (6)
N1	0.0213 (9)	0.0175 (9)	0.0244 (10)	0.0008 (7)	0.0076 (7)	0.0012 (7)
N2	0.0215 (8)	0.0118 (8)	0.0216 (9)	−0.0015 (7)	0.0079 (7)	−0.0002 (7)

N3	0.0201 (8)	0.0118 (9)	0.0222 (9)	−0.0008 (7)	0.0083 (7)	0.0008 (7)
N4	0.0206 (9)	0.0121 (9)	0.0205 (9)	−0.0013 (7)	0.0043 (7)	−0.0006 (7)
N5	0.0192 (8)	0.0178 (10)	0.0219 (9)	−0.0016 (7)	0.0027 (7)	0.0001 (7)
N6	0.0282 (10)	0.0216 (11)	0.0289 (11)	0.0028 (8)	0.0009 (9)	−0.0004 (8)
C1	0.0232 (11)	0.0216 (12)	0.0317 (13)	−0.0004 (9)	0.0076 (9)	0.0037 (10)
C2	0.0232 (11)	0.0310 (13)	0.0270 (12)	0.0045 (10)	0.0101 (9)	0.0016 (10)
C3	0.0310 (12)	0.0225 (12)	0.0220 (12)	0.0077 (10)	0.0065 (9)	−0.0023 (9)
C4	0.0244 (11)	0.0161 (11)	0.0231 (11)	0.0013 (9)	0.0042 (9)	−0.0005 (9)
C5	0.0204 (10)	0.0160 (11)	0.0206 (11)	0.0015 (8)	0.0032 (8)	0.0017 (8)
C6	0.0189 (10)	0.0122 (10)	0.0178 (10)	−0.0002 (8)	0.0028 (8)	0.0012 (8)
C7	0.0184 (9)	0.0122 (10)	0.0190 (10)	−0.0010 (8)	0.0037 (8)	0.0000 (8)
C8	0.0193 (10)	0.0173 (11)	0.0179 (11)	0.0000 (8)	0.0019 (8)	0.0024 (8)
C9	0.0245 (11)	0.0181 (11)	0.0242 (11)	−0.0022 (9)	0.0045 (9)	−0.0012 (9)
C10	0.0255 (11)	0.0229 (12)	0.0269 (12)	−0.0083 (9)	0.0023 (9)	0.0017 (10)
C11	0.0229 (11)	0.0317 (14)	0.0285 (12)	−0.0087 (10)	0.0078 (9)	0.0033 (10)
C12	0.0225 (11)	0.0279 (13)	0.0247 (11)	−0.0014 (10)	0.0071 (9)	−0.0013 (10)
C13	0.0248 (11)	0.0165 (11)	0.0274 (12)	−0.0013 (9)	0.0107 (10)	−0.0024 (9)
C14	0.0347 (13)	0.0219 (13)	0.0362 (14)	−0.0059 (11)	−0.0071 (11)	0.0029 (11)

Geometric parameters (Å, °)

Fe1—O1	2.160 (2)	C2—C3	1.380 (3)
Fe1—N1	2.289 (2)	C2—H2	0.9300
Fe1—N2	2.117 (2)	C3—C4	1.388 (3)
Fe1—N3^{i}	2.106 (2)	C3—H3	0.9300
Fe1—N5^{i}	2.303 (2)	C4—C5	1.383 (3)
Fe1—N6	2.059 (2)	C4—H4	0.9300
S1—C13	1.630 (2)	C5—C6	1.467 (3)
O1—C14	1.423 (3)	C7—C8	1.471 (3)
O1—H1o	0.82 (3)	C8—C9	1.385 (3)
N1—C1	1.335 (3)	C9—C10	1.386 (3)
N1—C5	1.362 (3)	C9—H9	0.9300
N2—C6	1.329 (3)	C10—C11	1.372 (3)
N2—N3	1.360 (2)	C10—H10	0.9300
N4—C6	1.357 (2)	C11—C12	1.394 (3)
N4—C7	1.359 (3)	C11—H11	0.9300
N5—C12	1.335 (3)	C12—H12	0.9300
N5—C8	1.356 (3)	C14—H14A	0.9600
N6—C13	1.158 (3)	C14—H14B	0.9600
C1—C2	1.390 (3)	C14—H14C	0.9600
C1—H1	0.9300		
N6—Fe1—N3^{i}	97.69 (7)	C2—C3—C4	118.9 (2)
N6—Fe1—N2	99.45 (7)	C2—C3—H3	120.5
N3^{i}—Fe1—N2	93.59 (6)	C4—C3—H3	120.5
N6—Fe1—O1	166.75 (7)	C5—C4—C3	118.93 (19)
N3^{i}—Fe1—O1	90.08 (6)	C5—C4—H4	120.5
N2—Fe1—O1	90.71 (6)	C3—C4—H4	120.5
N6—Fe1—N1	89.98 (7)	N1—C5—C4	122.55 (19)

$N3^{i}$—Fe1—N1	165.34 (6)	N1—C5—C6	113.25 (18)
N2—Fe1—N1	72.75 (6)	C4—C5—C6	124.20 (19)
O1—Fe1—N1	84.91 (6)	N2—C6—N4	113.04 (17)
N6—Fe1—$N5^{i}$	90.82 (7)	N2—C6—C5	117.38 (17)
$N3^{i}$—Fe1—$N5^{i}$	73.18 (6)	N4—C6—C5	129.58 (18)
N2—Fe1—$N5^{i}$	164.32 (6)	N3—C7—N4	112.96 (17)
O1—Fe1—$N5^{i}$	81.13 (6)	N3—C7—C8	117.37 (18)
N1—Fe1—$N5^{i}$	119.40 (6)	N4—C7—C8	129.61 (18)
C14—O1—Fe1	125.15 (14)	N5—C8—C9	122.85 (19)
C14—O1—H1o	109.9 (18)	N5—C8—C7	113.81 (18)
Fe1—O1—H1o	118.5 (19)	C9—C8—C7	123.32 (19)
C1—N1—C5	117.57 (18)	C8—C9—C10	118.6 (2)
C1—N1—Fe1	126.76 (15)	C8—C9—H9	120.7
C5—N1—Fe1	115.65 (13)	C10—C9—H9	120.7
C6—N2—N3	106.25 (16)	C11—C10—C9	119.2 (2)
C6—N2—Fe1	120.63 (13)	C11—C10—H10	120.4
N3—N2—Fe1	132.64 (13)	C9—C10—H10	120.4
C7—N3—N2	106.24 (16)	C10—C11—C12	118.9 (2)
C7—N3—$Fe1^{i}$	120.61 (13)	C10—C11—H11	120.6
N2—N3—$Fe1^{i}$	133.04 (13)	C12—C11—H11	120.6
C6—N4—C7	101.51 (16)	N5—C12—C11	123.0 (2)
C12—N5—C8	117.44 (19)	N5—C12—H12	118.5
C12—N5—$Fe1^{i}$	127.71 (15)	C11—C12—H12	118.5
C8—N5—$Fe1^{i}$	114.73 (13)	N6—C13—S1	178.7 (2)
C13—N6—Fe1	174.49 (19)	O1—C14—H14A	109.5
N1—C1—C2	123.1 (2)	O1—C14—H14B	109.5
N1—C1—H1	118.4	H14A—C14—H14B	109.5
C2—C1—H1	118.4	O1—C14—H14C	109.5
C3—C2—C1	118.9 (2)	H14A—C14—H14C	109.5
C3—C2—H2	120.5	H14B—C14—H14C	109.5
C1—C2—H2	120.5		
N6—Fe1—O1—C14	143.2 (3)	C1—N1—C5—C6	−179.54 (18)
$N3^{i}$—Fe1—O1—C14	−90.68 (18)	Fe1—N1—C5—C6	2.0 (2)
N2—Fe1—O1—C14	2.91 (18)	C3—C4—C5—N1	−1.0 (3)
N1—Fe1—O1—C14	75.52 (17)	C3—C4—C5—C6	179.54 (19)
$N5^{i}$—Fe1—O1—C14	−163.64 (18)	N3—N2—C6—N4	−0.3 (2)
N6—Fe1—N1—C1	−82.18 (18)	Fe1—N2—C6—N4	172.72 (12)
$N3^{i}$—Fe1—N1—C1	156.0 (2)	N3—N2—C6—C5	−179.34 (17)
N2—Fe1—N1—C1	177.91 (19)	Fe1—N2—C6—C5	−6.3 (2)
O1—Fe1—N1—C1	85.58 (18)	C7—N4—C6—N2	0.0 (2)
$N5^{i}$—Fe1—N1—C1	8.7 (2)	C7—N4—C6—C5	178.9 (2)
N6—Fe1—N1—C5	96.12 (15)	N1—C5—C6—N2	2.5 (3)
$N3^{i}$—Fe1—N1—C5	−25.7 (3)	C4—C5—C6—N2	−177.98 (19)
N2—Fe1—N1—C5	−3.79 (14)	N1—C5—C6—N4	−176.37 (19)
O1—Fe1—N1—C5	−96.12 (15)	C4—C5—C6—N4	3.2 (3)

N5^{i}—Fe1—N1—C5	−172.96 (13)	N2—N3—C7—N4	−0.5 (2)
N6—Fe1—N2—C6	−81.62 (16)	Fe1^{i}—N3—C7—N4	176.19 (13)
N3^{i}—Fe1—N2—C6	179.96 (16)	N2—N3—C7—C8	176.88 (16)
O1—Fe1—N2—C6	89.84 (16)	Fe1^{i}—N3—C7—C8	−6.4 (2)
N1—Fe1—N2—C6	5.39 (15)	C6—N4—C7—N3	0.3 (2)
N5^{i}—Fe1—N2—C6	148.1 (2)	C6—N4—C7—C8	−176.7 (2)
N6—Fe1—N2—N3	89.26 (18)	C12—N5—C8—C9	−0.4 (3)
N3^{i}—Fe1—N2—N3	−9.1 (2)	Fe1^{i}—N5—C8—C9	175.95 (16)
O1—Fe1—N2—N3	−99.28 (18)	C12—N5—C8—C7	−178.85 (17)
N1—Fe1—N2—N3	176.27 (19)	Fe1^{i}—N5—C8—C7	−2.5 (2)
N5^{i}—Fe1—N2—N3	−41.0 (3)	N3—C7—C8—N5	5.7 (3)
C6—N2—N3—C7	0.5 (2)	N4—C7—C8—N5	−177.49 (19)
Fe1—N2—N3—C7	−171.37 (14)	N3—C7—C8—C9	−172.74 (19)
C6—N2—N3—Fe1^{i}	−175.62 (14)	N4—C7—C8—C9	4.1 (3)
Fe1—N2—N3—Fe1^{i}	12.5 (3)	N5—C8—C9—C10	−1.3 (3)
C5—N1—C1—C2	0.1 (3)	C7—C8—C9—C10	176.91 (19)
Fe1—N1—C1—C2	178.33 (16)	C8—C9—C10—C11	1.6 (3)
N1—C1—C2—C3	−0.9 (3)	C9—C10—C11—C12	−0.1 (3)
C1—C2—C3—C4	0.9 (3)	C8—N5—C12—C11	2.0 (3)
C2—C3—C4—C5	0.0 (3)	Fe1^{i}—N5—C12—C11	−173.83 (16)
C1—N1—C5—C4	0.9 (3)	C10—C11—C12—N5	−1.8 (3)
Fe1—N1—C5—C4	−177.56 (16)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···N4^{ii}	0.82 (3)	1.89 (3)	2.698 (2)	169 (3)

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

Fig. 1