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fac-Bis[bis(pyridin-2-yl)methanamine]iron(II) bis(1,1,3,3-tetracyano-2-ethoxypropenide) dihydrate

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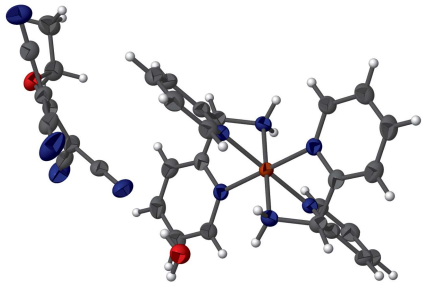
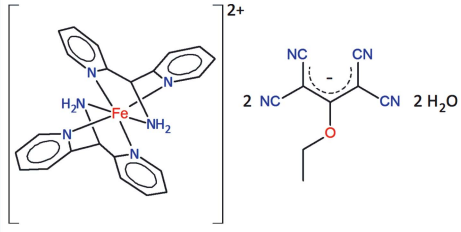
The hydrated complex $[Fe(DIPA)_2](tcnoet)_2\cdot 2H_2O$ [DIPA is bis(pyridin-2-yl)-methanamine, $C_{11}H_{11}N_3$, and tcnoet is the anion 1,1,3,3-tetracyano-2-ethoxy-propenide, $C_9H_5N_4O^-$], crystallizes with the $[Fe(DIPA)_2]^{2+}$ cation located on an inversion centre. The coordination geometry for Fe^{II} is strongly distorted from octahedral, as a consequence of the bite angles formed by the tridentate DIPA ligand. The water molecules included in the voids left by the cations and anions form hydrogen bonds with the cyano and amine groups.

3D view



Chemical scheme



Structure description

Polynitrile anions have recently received considerable attention in the fields of coordination chemistry and molecular materials (Benmansour *et al.*, 2010). These organic anions are of interest due to their ability to act towards metal atoms with various coordination modes and for their high degree of electronic delocalization (Yuste *et al.*, 2009; Atmani *et al.*, 2008; Benmansour *et al.*, 2008, 2012; Miyazaki *et al.*, 2003; Setifi, Domasevitch *et al.*, 2013; Setifi, Charles *et al.*, 2013; Setifi, Milin *et al.*, 2014; Setifi, Lehchili *et al.*, 2014; Setifi, Setifi *et al.*, 2014; Addala *et al.*, 2015).

We are interested in using these anionic ligands in combination with other neutral bridging co-ligands to explore their structural features and properties relevant to the field of molecular materials exhibiting the spin-crossover phenomenon. In an attempt to prepare such an iron(II) complex using hydrothermal synthesis, we obtained instead the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N15^{i}	0.86 (4)	2.12 (4)	2.976 (3)	172 (3)
O1—H2···N17	0.84 (4)	2.09 (4)	2.921 (3)	175 (4)
N2—H2B···O1^{ii}	0.91	2.25	3.065 (3)	149

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y+2, -z+1$.

In the title compound, the complex cation lies on an inversion centre, while the organic anion and the lattice water molecule are in general positions, giving the chemical formula $[Fe(DIPA)_2](tcnoet)_2{\cdot}2H_2O$, where DIPA is the tridentate amine ligand bis(pyridin-2-yl)methanamine and tcnoet is the anion 1,1,3,3-tetracyano-2-ethoxypropenide (Fig. 1). The tri-amine ligand displays a butterfly conformation, imposed by the sp^3 hybridization of the central C atom C6, giving a dihedral angle between the pyridyl rings of 75.87 (8)°. The three N donors coordinate in a *facial* arrangement, with very similar Fe—N bond lengths [range: 1.9904 (18)–2.0106 (19) Å]. However, the octahedral coordination geometry for the metal is strongly distorted as a consequence of the steric strain originating from the bite angles formed by the ligand in the five-membered metalacycles: N1—Fe1—N2 = 80.28 (8)° and N2—Fe1—N3 = 80.95 (8)°. Such a distortion has been observed in other octahedral complexes featuring this ligand with different transition metals (Fe^{II}, Co^{III}, Ni^{II}, Cu^{II}: Bernhardt *et al.*, 1992; Fe^{III}: Renz *et al.*, 1999; Mn^{II}: Bräuer *et al.*, 2011). Regarding the free anion tcnoet, its twisted conformation, characterized by a dihedral angle of 29.8 (2)° between the dicyano $C(CN)_2$ mean planes, is not uncommon, and is indeed comparable to that observed in the 2,2′-bipyridin-1-ium salt (Setifi *et al.*, 2015; dihedral angle: 22.4°).

The water molecule behaves both as donor and acceptor for hydrogen bonding, stabilizing the crystal structure with three weak hydrogen bonds involving two symmetry-related tcnoet anions and the central amine group of the DIPA ligand (Table 1 and Fig. 2).

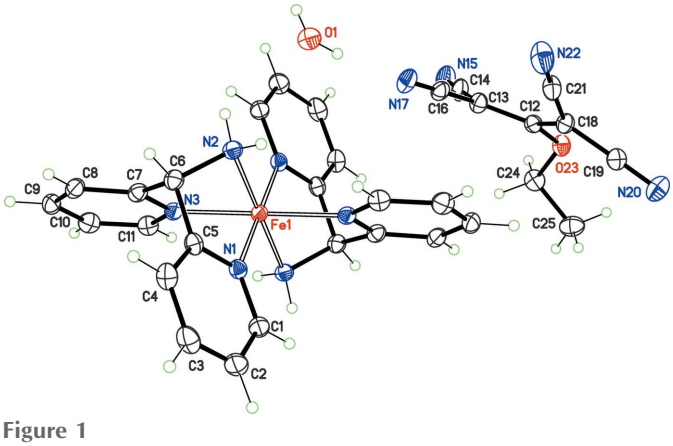


Figure 1
The structures of the molecular components in the title compound, with displacement ellipsoids drawn at the 30% probability level. Non-labelled atoms in the cation are generated by the symmetry operation $1-x, 1-y, 1-z$.

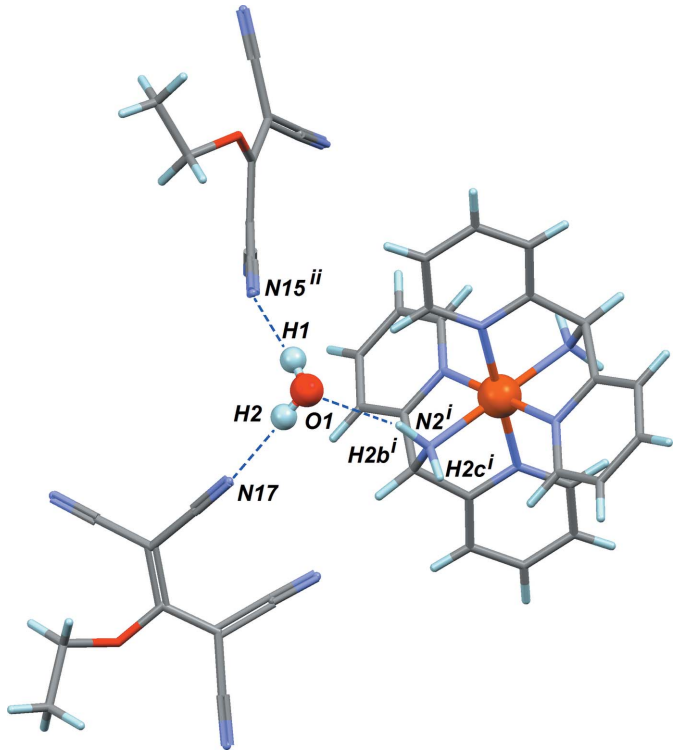


Figure 2
Part of the crystal structure, showing the hydrogen bonds formed by the water molecule (dashed lines). [Symmetry codes: i $1-x, 2-y, 1-z$; ii $1-x, \frac{1}{2}+y, \frac{3}{2}-z$.]

Synthesis and crystallization

The salt K(tcnoet) was prepared using the published method (Middleton *et al.*, 1958). The title compound was synthesized hydrothermally under autogenous pressure from a mixture of $FeSO_4{\cdot}7H_2O$ (28 mg, 0.1 mmol), DIPA (19 mg, 0.1 mmol) and K(tcnoet) (45 mg, 0.2 mmol) in water–methanol (4:1 *v*/*v*, 20 cm^3). This mixture was sealed in a Teflon-lined autoclave and held at 423 K for 3 days, and then cooled to ambient temperature at a rate of 10 K h^{-1} (yield: 23%). Red prisms of the title compound suitable for single-crystal X-ray diffraction were selected directly from the synthesized product.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Two reflections ($\bar{1}$ 9 1, $\bar{2}$ 9 1) were omitted because of poor agreement between calculated and observed intensities.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{11}H_{11}N_3)_2](C_9H_5N_4O)_2{\cdot}2H_2O$
M_r	832.68
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	11.8904 (3), 7.5824 (3), 22.5912 (7)
β (°)	102.648 (3)
V (Å^3)	1987.35 (11)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.55
Crystal size (mm)	0.12 × 0.08 × 0.07
Data collection	
Diffractometer	Agilent Xcalibur
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.843, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8154, 3799, 3393
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.115, 1.07
No. of reflections	3799
No. of parameters	275
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.32

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *XP* in *SHELXTL-Plus* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2017). **2**, x171007 [https://doi.org/10.1107/S2414314617010070]

fac-Bis[bis(pyridin-2-yl)methanamine]iron(II) bis(1,1,3,3-tetracyano-2-ethoxypropenide) dihydrate

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fac-Bis[bis(pyridin-2-yl)methanamine]iron(II) bis(1,1,3,3-tetracyano-2-ethoxypropenide) dihydrate

Crystal data

$[Fe(C_{11}H_{11}N_3)_2](C_9H_5N_4O)_2{\cdot}2H_2O$
M_r = 832.68
Monoclinic, $P2_1/c$
a = 11.8904 (3) Å
b = 7.5824 (3) Å
c = 22.5912 (7) Å
β = 102.648 (3)°
V = 1987.35 (11) Å^3
Z = 2
$F(000)$ = 864
D_x = 1.391 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3092 reflections
θ = 4.9–71.4°
μ = 3.55 mm^{-1}
T = 173 K
Prism, red
0.12 × 0.08 × 0.07 mm

Data collection

Agilent Xcalibur diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.843, T_{max} = 1.000
8154 measured reflections
3799 independent reflections
3393 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 71.5°, θ_{min} = 3.8°
h = −8→14
k = −9→9
l = −27→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.07
3799 reflections
275 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 1.1004P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Refinement. H atoms for the water molecule, H1 and H2, were found in a difference map and refined freely, while other H atoms were placed in calculated positions.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.500000	0.500000	0.500000	0.02633 (14)
N1	0.47707 (16)	0.5225 (2)	0.41019 (8)	0.0283 (4)
N2	0.58098 (16)	0.7306 (3)	0.49521 (8)	0.0303 (4)
H2B	0.530419	0.819642	0.481911	0.036*
H2C	0.627271	0.760881	0.531435	0.036*
N3	0.65696 (15)	0.4086 (3)	0.50006 (8)	0.0287 (4)
C1	0.3948 (2)	0.4541 (3)	0.36576 (11)	0.0349 (5)
H1A	0.334845	0.386283	0.376208	0.042*
C2	0.3951 (2)	0.4799 (4)	0.30524 (11)	0.0428 (6)
H2A	0.336248	0.429819	0.274536	0.051*
C3	0.4821 (2)	0.5793 (4)	0.28976 (11)	0.0448 (6)
H3A	0.484164	0.597059	0.248387	0.054*
C4	0.5656 (2)	0.6523 (4)	0.33527 (11)	0.0381 (5)
H4A	0.625319	0.722921	0.325822	0.046*
C5	0.56069 (18)	0.6207 (3)	0.39475 (10)	0.0300 (5)
C6	0.64886 (19)	0.6820 (3)	0.44945 (10)	0.0317 (5)
H6A	0.697765	0.781002	0.440069	0.038*
C7	0.71790 (19)	0.5212 (3)	0.47388 (10)	0.0305 (5)
C8	0.82888 (19)	0.4864 (3)	0.46739 (11)	0.0339 (5)
H8A	0.869537	0.569249	0.448410	0.041*
C9	0.8789 (2)	0.3285 (4)	0.48920 (11)	0.0374 (5)
H9A	0.955088	0.300655	0.485800	0.045*
C10	0.8163 (2)	0.2115 (4)	0.51606 (11)	0.0389 (5)
H10A	0.848966	0.101461	0.530923	0.047*
C11	0.7063 (2)	0.2551 (3)	0.52122 (10)	0.0344 (5)
H11A	0.664212	0.174451	0.540237	0.041*
C12	0.09125 (19)	0.7045 (3)	0.67459 (10)	0.0304 (5)
C13	0.21113 (19)	0.6807 (3)	0.69238 (10)	0.0337 (5)
C14	0.2614 (2)	0.5841 (4)	0.74535 (11)	0.0397 (6)
N15	0.3030 (2)	0.5080 (4)	0.78845 (11)	0.0539 (7)
C16	0.28834 (19)	0.7605 (3)	0.66036 (10)	0.0343 (5)
N17	0.35231 (17)	0.8214 (3)	0.63518 (10)	0.0431 (5)
C18	0.03496 (19)	0.8350 (3)	0.63568 (10)	0.0319 (5)
C19	−0.0856 (2)	0.8176 (3)	0.61052 (11)	0.0359 (5)
N20	−0.18179 (19)	0.8052 (3)	0.58885 (11)	0.0495 (6)
C21	0.0890 (2)	0.9891 (3)	0.61936 (13)	0.0406 (6)
N22	0.1294 (2)	1.1153 (4)	0.60585 (15)	0.0630 (8)
O23	0.01861 (14)	0.5995 (2)	0.69608 (8)	0.0359 (4)
C24	0.0371 (2)	0.4105 (4)	0.70181 (12)	0.0420 (6)
H24A	0.066260	0.377862	0.744869	0.050*
H24B	0.093996	0.372397	0.678350	0.050*
C25	−0.0772 (3)	0.3253 (4)	0.67742 (14)	0.0521 (7)
H25A	−0.069029	0.196912	0.681080	0.078*
H25B	−0.104317	0.357179	0.634632	0.078*
H25C	−0.132936	0.365979	0.700568	0.078*

O1	0.54085 (17)	0.9789 (3)	0.58946 (8)	0.0392 (4)
H1	0.591 (3)	0.990 (4)	0.6229 (18)	0.059*
H2	0.487 (3)	0.928 (5)	0.6009 (16)	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0235 (2)	0.0339 (3)	0.0221 (2)	−0.0020 (2)	0.00606 (17)	−0.0021 (2)
N1	0.0273 (9)	0.0310 (10)	0.0267 (9)	0.0039 (7)	0.0060 (7)	0.0008 (7)
N2	0.0303 (9)	0.0317 (10)	0.0284 (9)	−0.0034 (8)	0.0053 (7)	−0.0018 (8)
N3	0.0269 (8)	0.0354 (10)	0.0237 (8)	−0.0022 (8)	0.0051 (7)	−0.0026 (8)
C1	0.0321 (11)	0.0411 (13)	0.0302 (11)	0.0022 (10)	0.0040 (9)	−0.0021 (10)
C2	0.0405 (13)	0.0561 (17)	0.0284 (12)	0.0081 (12)	0.0005 (10)	−0.0026 (11)
C3	0.0489 (14)	0.0619 (18)	0.0246 (11)	0.0167 (13)	0.0101 (10)	0.0075 (11)
C4	0.0367 (12)	0.0447 (14)	0.0349 (12)	0.0072 (11)	0.0118 (10)	0.0113 (11)
C5	0.0308 (10)	0.0299 (11)	0.0305 (11)	0.0066 (9)	0.0096 (9)	0.0051 (9)
C6	0.0316 (10)	0.0313 (12)	0.0333 (11)	−0.0043 (9)	0.0098 (9)	0.0015 (9)
C7	0.0294 (11)	0.0352 (12)	0.0261 (10)	−0.0040 (9)	0.0041 (9)	0.0004 (9)
C8	0.0277 (11)	0.0425 (14)	0.0309 (11)	−0.0053 (10)	0.0050 (9)	−0.0002 (10)
C9	0.0280 (10)	0.0495 (15)	0.0331 (12)	0.0044 (10)	0.0035 (9)	−0.0044 (11)
C10	0.0408 (12)	0.0390 (13)	0.0334 (12)	0.0058 (11)	0.0004 (10)	0.0033 (10)
C11	0.0390 (12)	0.0353 (13)	0.0282 (10)	−0.0003 (10)	0.0058 (9)	0.0045 (10)
C12	0.0309 (10)	0.0350 (12)	0.0272 (10)	−0.0021 (9)	0.0101 (9)	−0.0021 (9)
C13	0.0310 (11)	0.0423 (14)	0.0287 (11)	0.0007 (10)	0.0085 (9)	0.0036 (10)
C14	0.0297 (11)	0.0538 (16)	0.0372 (13)	0.0040 (11)	0.0109 (10)	0.0052 (12)
N15	0.0409 (12)	0.0785 (19)	0.0416 (13)	0.0115 (12)	0.0074 (10)	0.0193 (13)
C16	0.0280 (10)	0.0444 (14)	0.0284 (11)	−0.0005 (10)	0.0013 (9)	−0.0008 (10)
N17	0.0291 (9)	0.0625 (15)	0.0378 (11)	−0.0054 (10)	0.0074 (9)	0.0055 (10)
C18	0.0286 (10)	0.0354 (13)	0.0329 (11)	−0.0019 (9)	0.0093 (9)	0.0031 (10)
C19	0.0368 (13)	0.0357 (13)	0.0354 (12)	0.0031 (10)	0.0084 (10)	0.0055 (10)
N20	0.0375 (12)	0.0540 (15)	0.0526 (13)	−0.0038 (10)	0.0006 (10)	0.0110 (12)
C21	0.0349 (12)	0.0391 (14)	0.0515 (15)	0.0061 (11)	0.0174 (11)	0.0070 (12)
N22	0.0562 (14)	0.0428 (14)	0.102 (2)	0.0016 (12)	0.0435 (15)	0.0168 (15)
O23	0.0346 (8)	0.0367 (9)	0.0398 (9)	0.0000 (7)	0.0156 (7)	0.0070 (7)
C24	0.0467 (14)	0.0387 (14)	0.0432 (14)	−0.0013 (11)	0.0156 (11)	0.0057 (11)
C25	0.0606 (17)	0.0489 (17)	0.0465 (15)	−0.0134 (14)	0.0112 (13)	−0.0009 (13)
O1	0.0429 (10)	0.0412 (10)	0.0338 (9)	−0.0055 (8)	0.0094 (8)	0.0029 (8)

Geometric parameters (Å, º)

Fe1—N3^{i}	1.9904 (18)	C8—H8A	0.9500
Fe1—N3	1.9904 (18)	C9—C10	1.380 (4)
Fe1—N1^{i}	1.9944 (18)	C9—H9A	0.9500
Fe1—N1	1.9944 (18)	C10—C11	1.379 (3)
Fe1—N2^{i}	2.0106 (19)	C10—H10A	0.9500
Fe1—N2	2.0106 (19)	C11—H11A	0.9500
N1—C1	1.343 (3)	C12—O23	1.341 (3)
N1—C5	1.348 (3)	C12—C18	1.393 (3)

N2—C6	1.490 (3)	C12—C13	1.405 (3)
N2—H2B	0.9100	C13—C14	1.418 (3)
N2—H2C	0.9100	C13—C16	1.423 (3)
N3—C7	1.338 (3)	C14—N15	1.147 (3)
N3—C11	1.343 (3)	C16—N17	1.142 (3)
C1—C2	1.382 (3)	C18—C21	1.420 (3)
C1—H1A	0.9500	C18—C19	1.428 (3)
C2—C3	1.385 (4)	C19—N20	1.145 (3)
C2—H2A	0.9500	C21—N22	1.142 (4)
C3—C4	1.379 (4)	O23—C24	1.451 (3)
C3—H3A	0.9500	C24—C25	1.496 (4)
C4—C5	1.379 (3)	C24—H24A	0.9900
C4—H4A	0.9500	C24—H24B	0.9900
C5—C6	1.508 (3)	C25—H25A	0.9800
C6—C7	1.506 (3)	C25—H25B	0.9800
C6—H6A	1.0000	C25—H25C	0.9800
C7—C8	1.385 (3)	O1—H1	0.86 (4)
C8—C9	1.379 (4)	O1—H2	0.84 (4)

$N3^{i}$—Fe1—N3	180.0	N2—C6—H6A	112.9
$N3^{i}$—Fe1—$N1^{i}$	87.13 (7)	C7—C6—H6A	112.9
N3—Fe1—$N1^{i}$	92.87 (7)	C5—C6—H6A	112.9
$N3^{i}$—Fe1—N1	92.88 (7)	N3—C7—C8	123.1 (2)
N3—Fe1—N1	87.13 (7)	N3—C7—C6	111.96 (19)
$N1^{i}$—Fe1—N1	180.0	C8—C7—C6	124.8 (2)
$N3^{i}$—Fe1—$N2^{i}$	80.95 (8)	C9—C8—C7	118.3 (2)
N3—Fe1—$N2^{i}$	99.05 (8)	C9—C8—H8A	120.9
$N1^{i}$—Fe1—$N2^{i}$	80.28 (8)	C7—C8—H8A	120.9
N1—Fe1—$N2^{i}$	99.72 (8)	C8—C9—C10	118.9 (2)
$N3^{i}$—Fe1—N2	99.05 (8)	C8—C9—H9A	120.5
N3—Fe1—N2	80.95 (8)	C10—C9—H9A	120.5
$N1^{i}$—Fe1—N2	99.72 (8)	C11—C10—C9	119.7 (2)
N1—Fe1—N2	80.27 (8)	C11—C10—H10A	120.1
$N2^{i}$—Fe1—N2	180.0	C9—C10—H10A	120.1
C1—N1—C5	118.5 (2)	N3—C11—C10	121.7 (2)
C1—N1—Fe1	129.96 (16)	N3—C11—H11A	119.1
C5—N1—Fe1	111.50 (15)	C10—C11—H11A	119.1
C6—N2—Fe1	99.26 (13)	O23—C12—C18	113.05 (19)
C6—N2—H2B	111.9	O23—C12—C13	120.9 (2)
Fe1—N2—H2B	111.9	C18—C12—C13	126.1 (2)
C6—N2—H2C	111.9	C12—C13—C14	121.4 (2)
Fe1—N2—H2C	111.9	C12—C13—C16	121.8 (2)
H2B—N2—H2C	109.6	C14—C13—C16	116.7 (2)
C7—N3—C11	118.26 (19)	N15—C14—C13	179.0 (3)
C7—N3—Fe1	112.10 (16)	N17—C16—C13	178.3 (3)
C11—N3—Fe1	129.63 (16)	C12—C18—C21	124.5 (2)
N1—C1—C2	121.7 (2)	C12—C18—C19	119.2 (2)
N1—C1—H1A	119.1	C21—C18—C19	116.4 (2)

C2—C1—H1A	119.1	N20—C19—C18	178.1 (3)
C1—C2—C3	119.4 (2)	N22—C21—C18	178.0 (3)
C1—C2—H2A	120.3	C12—O23—C24	121.45 (18)
C3—C2—H2A	120.3	O23—C24—C25	106.6 (2)
C4—C3—C2	119.1 (2)	O23—C24—H24A	110.4
C4—C3—H3A	120.5	C25—C24—H24A	110.4
C2—C3—H3A	120.5	O23—C24—H24B	110.4
C5—C4—C3	118.6 (2)	C25—C24—H24B	110.4
C5—C4—H4A	120.7	H24A—C24—H24B	108.6
C3—C4—H4A	120.7	C24—C25—H25A	109.5
N1—C5—C4	122.7 (2)	C24—C25—H25B	109.5
N1—C5—C6	112.21 (19)	H25A—C25—H25B	109.5
C4—C5—C6	125.1 (2)	C24—C25—H25C	109.5
N2—C6—C7	106.29 (18)	H25A—C25—H25C	109.5
N2—C6—C5	105.05 (17)	H25B—C25—H25C	109.5
C7—C6—C5	106.01 (19)	H1—O1—H2	102 (3)

C5—N1—C1—C2	1.0 (3)	C5—C6—C7—N3	−71.4 (2)
Fe1—N1—C1—C2	−177.85 (19)	N2—C6—C7—C8	−143.5 (2)
N1—C1—C2—C3	−0.3 (4)	C5—C6—C7—C8	105.0 (2)
C1—C2—C3—C4	−0.8 (4)	N3—C7—C8—C9	−0.2 (4)
C2—C3—C4—C5	1.2 (4)	C6—C7—C8—C9	−176.3 (2)
C1—N1—C5—C4	−0.6 (3)	C7—C8—C9—C10	0.5 (3)
Fe1—N1—C5—C4	178.47 (18)	C8—C9—C10—C11	−0.7 (4)
C1—N1—C5—C6	−177.8 (2)	C7—N3—C11—C10	−0.5 (3)
Fe1—N1—C5—C6	1.2 (2)	Fe1—N3—C11—C10	178.39 (17)
C3—C4—C5—N1	−0.5 (4)	C9—C10—C11—N3	0.8 (4)
C3—C4—C5—C6	176.3 (2)	O23—C12—C13—C14	−18.8 (4)
Fe1—N2—C6—C7	−55.23 (17)	C18—C12—C13—C14	159.7 (3)
Fe1—N2—C6—C5	56.87 (17)	O23—C12—C13—C16	165.0 (2)
N1—C5—C6—N2	−40.1 (2)	C18—C12—C13—C16	−16.5 (4)
C4—C5—C6—N2	142.7 (2)	O23—C12—C18—C21	162.7 (2)
N1—C5—C6—C7	72.2 (2)	C13—C12—C18—C21	−15.9 (4)
C4—C5—C6—C7	−105.0 (3)	O23—C12—C18—C19	−16.3 (3)
C11—N3—C7—C8	0.3 (3)	C13—C12—C18—C19	165.1 (2)
Fe1—N3—C7—C8	−178.85 (18)	C18—C12—O23—C24	139.3 (2)
C11—N3—C7—C6	176.80 (19)	C13—C12—O23—C24	−42.0 (3)
Fe1—N3—C7—C6	−2.3 (2)	C12—O23—C24—C25	−135.0 (2)
N2—C6—C7—N3	40.0 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N15^{ii}	0.86 (4)	2.12 (4)	2.976 (3)	172 (3)
O1—H2···N17	0.84 (4)	2.09 (4)	2.921 (3)	175 (4)
N2—H2*B*···O1^{iii}	0.91	2.25	3.065 (3)	149

N2—H2*C*···N20^{iv}	0.91	2.38	3.184 (3)	148
N2—H2*C*···O1	0.91	2.47	2.958 (3)	114

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