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Tris(2,2′-bipyridine)iron(II) tris(dicyanomethylidene)methanediide

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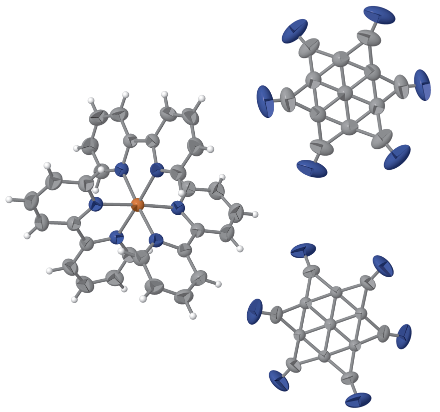
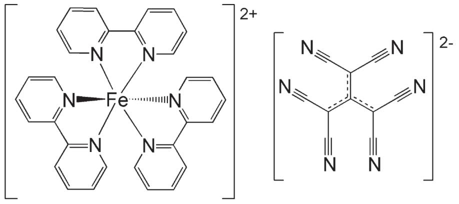
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $[Fe(C_{10}H_8N_2)_3][C\{C(CN)_2\}_3]$, contains an iron–bipyridyl unit and one third of two crystallographic independent tris(dicyanomethylidene)methanediide units. As a result of crystallographic site symmetry the ratio of cations to anions is 1:1. The tris(2,2′-bipyridine)iron(II) cation has threefold symmetry. The two crystallographic independent tris(dicyanomethylidene)methanediide ions are disordered over two atomic sites having equal occupancy. The anions have $\overline{3}$ symmetry. In the crystal, hydrogen bonds between cations and anions form complex layers parallel to (001). These are supplemented by hydrogen bonds perpendicular to the former, leading to a three-dimensional network.

3D view



Chemical scheme



Structure description

Organic cyanocarbanion anions have recently attracted considerable attention in the fields of coordination chemistry and molecular materials (Benmansour *et al.*, 2010). As a consequence of their rigidity and electronic delocalization, these organic anions provide opportunities for the generation of molecular architectures with varying dimensions and topologies (Benmansour *et al.*, 2008; Setifi *et al.*, 2010; Benamara *et al.*, 2021). Furthermore, the use of cyanocarbanion anions for the synthesis of interesting discrete and polymeric bistable materials has been recently reported (Setifi, Milin *et al.*, 2014; Cuza *et al.*, 2021). It was during the course of attempts to prepare such materials with 2,2′-bipyridine as a co-ligand that the title complex was unexpectedly obtained. We report here the molecular and supramolecular structures of a new compound based on tris(2,2′-bipyridine)iron(II) and the tris(dicyanomethylidene)methanediide dianion (tcpd^{2-}) as the counter-ion.

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Table 1
Selected geometric parameters (Å, °).

Fe1—N1	1.9688 (13)	C13—N3	1.067 (2)
Fe1—N2	1.9734 (13)	C14—C15	1.421 (3)
C11—C12	1.422 (3)	C15—C16	1.482 (4)
C12—C13	1.473 (3)	C16—N4	1.079 (3)
$N1^{i}$—Fe1—N1	96.73 (5)	N1—Fe1—N2	81.40 (5)
$N1^{i}$—Fe1—N2	85.75 (5)	N2—Fe1—$N2^{i}$	96.18 (5)
$N1^{ii}$—Fe1—N2	177.07 (5)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···$N1^{ii}$	0.93	2.61	3.121 (2)	115
C10—H10···$N2^{i}$	0.93	2.60	3.116 (2)	115
C4—H4···$N3^{iii}$	0.93	2.45	3.333 (3)	159
C8—H8···$N3^{iv}$	0.93	2.68	3.476 (3)	144
C3—H3···$N4^{iii}$	0.93	2.65	3.244 (3)	122
C10—H10···$N4^{v}$	0.93	2.68	3.437 (3)	139

Symmetry codes: (i) $-y+2, x-y+1, z$; (ii) $-x+y+1, -x+2, z$; (iii) $-y+1, x-y+1, z$; (iv) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{1}{3}$; (v) $-y+\frac{4}{3}, x-y+\frac{2}{3}, z-\frac{1}{3}$.

The crystal structure consists of an $[Fe(C_{10}H_8N_2)_3]^{2+}$ cation with a six-coordinate iron atom in a slightly distorted octahedral coordination environment and a $[C\{C(CN)_2\}_3]^{2-}$ anion (Fig. 1). At first glance, it is noticeable that two crystallographically independent anions are present. These have a site symmetry of $\overline{3}$, which means that one sixth is present in the asymmetric unit. The cation has site symmetry 3, *i.e.* it consists of an iron bipyridyl unit, with one third of the cation in the asymmetric unit. The resulting ratio of cation to anion is therefore 1:1. The two crystallographic independent tris(dicyanomethylidene)methanediide ions are disordered over two atomic sites having equal occupancy, leading to a star-like appearance.

The Fe—N distances are comparable to other tris(2,2′-bipyridine)iron(II) complexes (Healy *et al.*, 1983; Setifi, Setifi *et al.*, 2014; Addala *et al.*, 2018). The angle N1—Fe1—N2 [81.40 (5)°] is determined by the bite angle of the bipyridine unit. The other *cis* angles in the coordination polyhedron deviate from 90° (see Table 1), as the octahedral cation is subject to compression in the direction of the threefold rotation axis.

The tris(dicyanomethylidene)methanediide dianions are disordered at the methylidene carbon atoms C12 and C15. The cyano end groups C13—N3 and C16—N4 show slightly elongated displacement ellipsoids due to the disorder at the neighbouring atoms. The cores of the anions (atoms C11/C12 and C14/C15 with their symmetry equivalents, respectively) are exactly planar. The cyano groups are twisted out of these planes (Fig. 2), making dihedral angles with it of 28.0 (2)° (N3, C13, C12, C13*C*, N3*C*) and 29.6 (2)° (N4, C16, C15, C16*E*, N4*E*). This type of distortion has been observed before (Setifi *et al.*, 2018, 2020).

Intramolecular hydrogen bonds in the tris(2,2′-bipyridine)iron(II) cation are C1—H1···N1 and

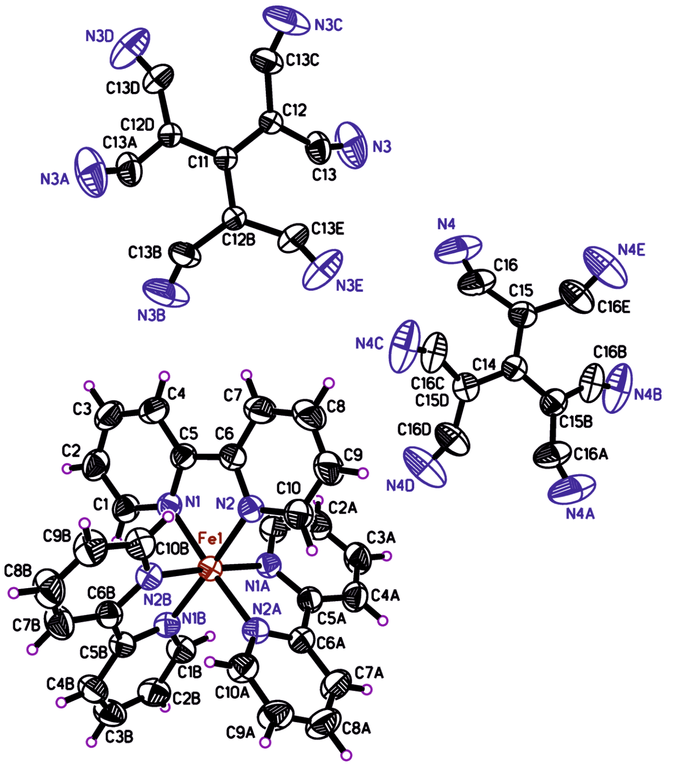

Figure 1
Molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn with 50% probability displacement ellipsoids. Only one of the disordered set of sites is shown.

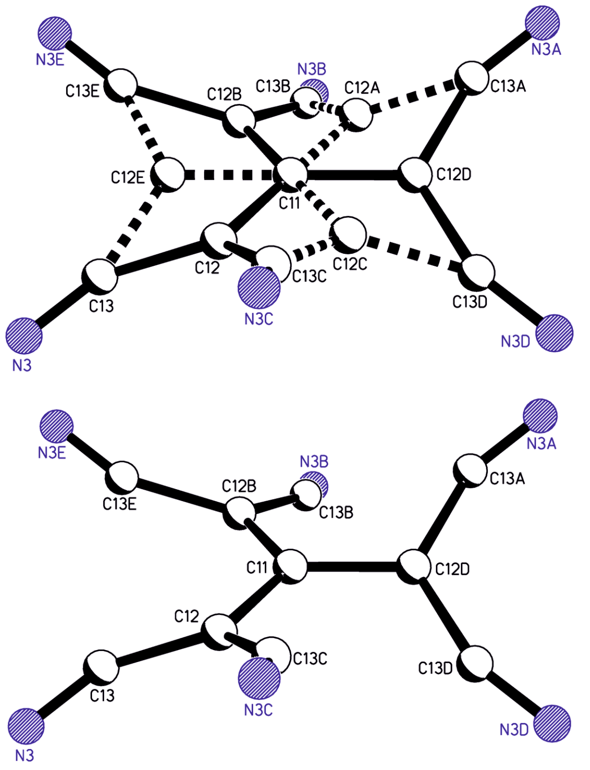

Figure 2
Side view of the anion C11—C12—C13—N3 with all symmetry-equivalent atoms (top). One of the two orientations is drawn with dashed bonds. Side view with one part of the disordered anion (bottom).

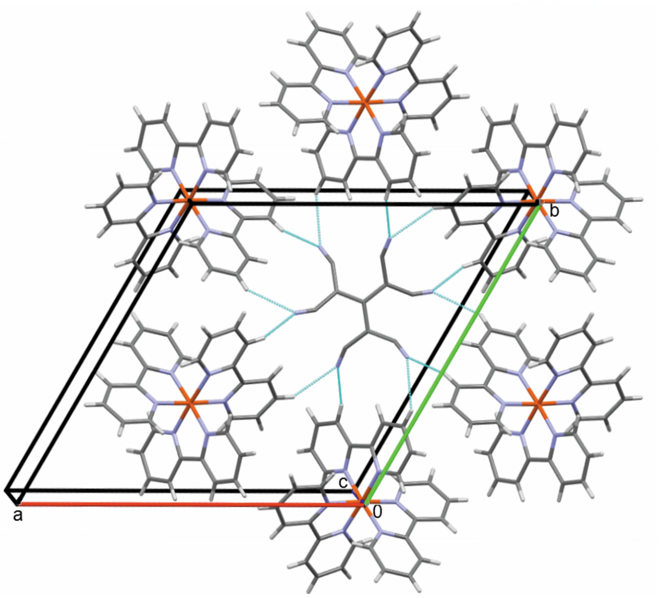

Figure 3
Partial packing diagram showing the hydrogen-bonding interactions C4—H4···N3 and C8—H8···N3 parallel to (001), as turquoise lines. Only one of the disordered set of sites is shown.

C10—H10···N2 between hydrogen atoms in *ortho* position and nitrogen atoms from neighbouring dipyridine units (Table 2). Further hydrogen bonds are present between cation and the anion consisting of C11—C12—C13—N3 with C4—H4···N3 and C8—H8···N3, which form complex layers parallel to (001) (Fig. 3). The other anion consisting of C14—C15—C16—N4 forms hydrogen bonds C3—H3···N4, forming layers that are also parallel to (001) (Fig. 4). Perpendicular to that are hydrogen bonds C10—H10···N4, which link the anion to two cations perpendicular to (001) (Fig. 5). All these interactions consolidate the crystal in a three-dimensional network of hydrogen bonds.

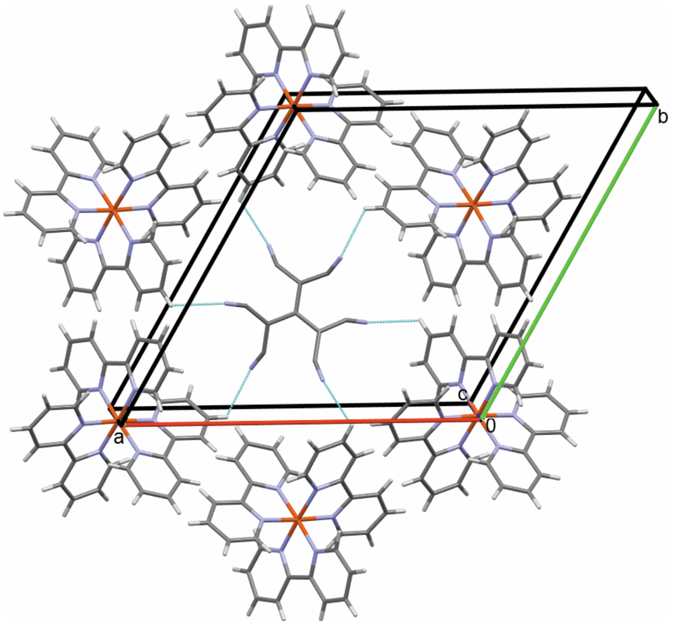

Figure 4
Partial packing diagram showing the hydrogen-bonding interactions C3—H3···N4 parallel to (001) as turquoise lines.. Only one of the disordered set of sites is shown.

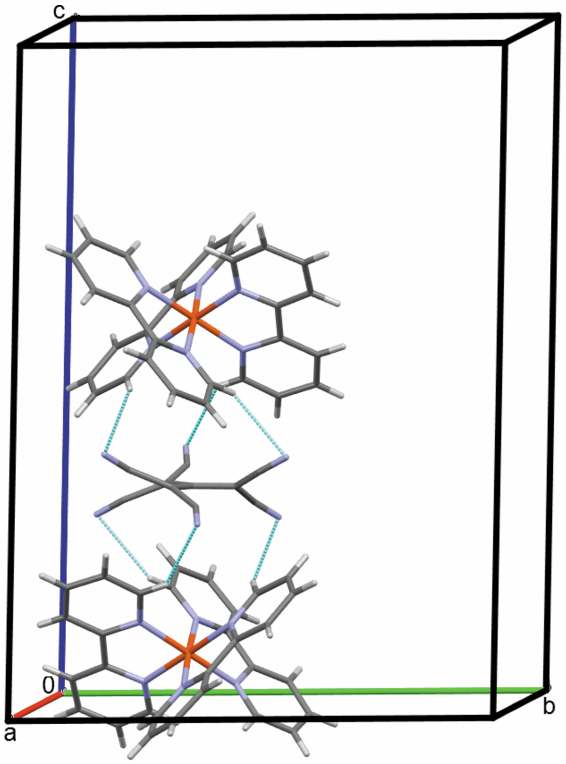

Figure 5
Partial packing diagram showing the hydrogen-bonding interactions C10—H10···N4 parallel to the crystallographic *c* axis, as turquoise lines. Only one of the disordered set of sites is shown.

There are more than 100 crystal structures of tris(2,2′-bipyridine)iron(II) complexes listed in the Cambridge Structural Database (Groom *et al.*, 2016). From these are five crystal structures of closely related complexes containing the tris(2,2′-bipyridine)iron(II) cation and different polynitrile anions (Setifi, Setifi *et al.*, 2014; Potočňák *et al.*, 2014; Potočňák & Váhovská, 2014; Addala *et al.*, 2018).

Synthesis and crystallization

A mixture of iron(II) bis(tetrafluoroborate) hexahydrate (34 mg, 0.1 mmol), 2,2′-dipyridyl (16 mg, 0.1 mmol) and dipotassium tris(dicyanomethylidene)methanediide (28 mg, 0.1 mmol), *N*,*N*-dimethylformamide (4 ml) and water (2 ml) was sonicated for 30 min. Then the reaction mixture was transferred to a Teflon-lined stainless steel reactor and placed in an oven. Subsequently, the temperature was kept 393 K for 3 days. After cooling to room temperature at a rate of 10 K h^{-1}, red plate-shaped crystals of the title compound were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The two crystallographic independent tris(dicyanomethylidene)methanediide ions are disordered over two atomic sites having equal occupancy.

Acknowledgements

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{10}H_8N_2)_3](C_{10}N_6)$
M_r	728.56
Crystal system, space group	Trigonal, $R\overline{3}:H$
Temperature (K)	298
a, c (Å)	17.0276 (3), 21.6388 (5)
V (Å^3)	5433.4 (2)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.46
Crystal size (mm)	0.45 × 0.28 × 0.15
Data collection	
Diffractometer	Bruker D8 VENTURE Duo
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.875, 0.922
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32654, 2780, 2269
R_{int}	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.091, 1.05
No. of reflections	2780
No. of parameters	170
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.35

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* (Farrugia, 2012).

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full crystallographic data

IUCrData (2025). **10**, x250503 [https://doi.org/10.1107/S2414314625005036]

Tris(2,2′-bipyridine)iron(II) tris(dicyanomethylidene)methanediide

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Tris(2,2′-bipyridine)iron(II) tris(dicyanomethylidene)methanediide

Crystal data

$[Fe(C_{10}H_8N_2)_3](C_{10}N_6)$
$M_r = 728.56$
Trigonal, $R\bar{3}:H$
$a = 17.0276$ (3) Å
$c = 21.6388$ (5) Å
$V = 5433.4$ (2) Å^3
$Z = 6$
$F(000) = 2244$

$D_x = 1.336$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5342 reflections
$\theta = 2.8$–$28.4°$
$\mu = 0.46$ mm^{-1}
$T = 298$ K
Plate, red
0.45 × 0.28 × 0.15 mm

Data collection

Bruker D8 VENTURE Duo diffractometer
Radiation source: sealed tube
TRIUMPH graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.875$, $T_{max} = 0.922$

32654 measured reflections
2780 independent reflections
2269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -22 \rightarrow 22$
$k = -22 \rightarrow 22$
$l = -28 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.091$
$S = 1.05$
2780 reflections
170 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 5.2576P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in idealized positions and refined with a riding model with C–H = 0.93 Å and with $U_{iso}(H) = 1.2\ U_{eq}(C)$.

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Fe1	1.000000	1.000000	0.24788 (2)	0.03504 (12)	
N1	0.89912 (9)	0.99778 (9)	0.29384 (6)	0.0386 (3)	
N2	0.89822 (9)	0.90276 (9)	0.20124 (5)	0.0391 (3)	
C1	0.90642 (12)	1.05483 (12)	0.33947 (7)	0.0475 (4)	
H1	0.963517	1.093679	0.355820	0.057*	
C2	0.83306 (13)	1.05808 (13)	0.36290 (8)	0.0562 (5)	
H2	0.840747	1.098700	0.394234	0.067*	
C3	0.74830 (13)	1.00060 (14)	0.33947 (9)	0.0590 (5)	
H3	0.697874	1.002039	0.354509	0.071*	
C4	0.73902 (12)	0.94059 (13)	0.29322 (9)	0.0536 (4)	
H4	0.682084	0.900635	0.277093	0.064*	
C5	0.81535 (11)	0.94053 (11)	0.27110 (7)	0.0408 (3)	
C6	0.81457 (11)	0.88191 (11)	0.22107 (7)	0.0423 (3)	
C7	0.73688 (13)	0.81059 (13)	0.19582 (9)	0.0593 (5)	
H7	0.679985	0.798009	0.209532	0.071*	
C8	0.74465 (14)	0.75829 (14)	0.15005 (10)	0.0685 (6)	
H8	0.693155	0.709862	0.132822	0.082*	
C9	0.82930 (14)	0.77881 (13)	0.13043 (9)	0.0609 (5)	
H9	0.836022	0.744194	0.099887	0.073*	
C10	0.90415 (12)	0.85113 (12)	0.15642 (7)	0.0491 (4)	
H10	0.961322	0.865004	0.142456	0.059*	
C11	0.333333	0.666667	0.166667	0.0315 (7)	
C12	0.27300 (19)	0.57138 (18)	0.16798 (14)	0.0356 (6)	0.5
C13	0.30840 (13)	0.51355 (11)	0.19074 (8)	0.0512 (4)	
N3	0.29929 (17)	0.45296 (12)	0.21194 (10)	0.0919 (7)	
C14	0.666667	0.333333	0.333333	0.0427 (8)	
C15	0.5716 (2)	0.2721 (3)	0.33372 (16)	0.0504 (8)	0.5
C16	0.51371 (14)	0.30692 (18)	0.35854 (9)	0.0707 (6)	
N4	0.45347 (15)	0.2971 (2)	0.38184 (11)	0.1096 (9)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.03581 (14)	0.03581 (14)	0.03350 (19)	0.01790 (7)	0.000	0.000
N1	0.0407 (7)	0.0398 (7)	0.0371 (6)	0.0215 (6)	−0.0010 (5)	−0.0020 (5)
N2	0.0416 (7)	0.0391 (7)	0.0361 (6)	0.0199 (6)	0.0000 (5)	−0.0012 (5)
C1	0.0495 (9)	0.0523 (10)	0.0438 (8)	0.0277 (8)	−0.0018 (7)	−0.0088 (7)
C2	0.0636 (11)	0.0616 (11)	0.0539 (10)	0.0391 (10)	0.0022 (9)	−0.0113 (8)
C3	0.0543 (11)	0.0693 (12)	0.0665 (11)	0.0408 (10)	0.0069 (9)	−0.0051 (9)
C4	0.0417 (9)	0.0602 (11)	0.0618 (10)	0.0277 (8)	−0.0010 (8)	−0.0054 (8)
C5	0.0399 (8)	0.0422 (8)	0.0423 (8)	0.0220 (7)	−0.0005 (6)	−0.0001 (6)
C6	0.0404 (8)	0.0414 (8)	0.0440 (8)	0.0196 (7)	−0.0028 (6)	−0.0026 (6)
C7	0.0424 (9)	0.0580 (11)	0.0672 (11)	0.0174 (9)	−0.0047 (8)	−0.0150 (9)
C8	0.0539 (11)	0.0600 (12)	0.0746 (13)	0.0158 (10)	−0.0121 (10)	−0.0258 (10)
C9	0.0646 (12)	0.0551 (11)	0.0564 (10)	0.0251 (9)	−0.0038 (9)	−0.0197 (9)

C10	0.0497 (9)	0.0508 (10)	0.0441 (8)	0.0231 (8)	0.0011 (7)	−0.0086 (7)
C11	0.0298 (10)	0.0298 (10)	0.0348 (16)	0.0149 (5)	0.000	0.000
C12	0.0305 (13)	0.0306 (14)	0.0452 (15)	0.0148 (11)	−0.0008 (12)	−0.0012 (11)
C13	0.0638 (11)	0.0358 (8)	0.0563 (10)	0.0267 (8)	−0.0048 (8)	0.0013 (7)
N3	0.133 (2)	0.0465 (10)	0.0953 (14)	0.0447 (12)	−0.0088 (14)	0.0143 (10)
C14	0.0450 (13)	0.0450 (13)	0.0380 (18)	0.0225 (6)	0.000	0.000
C15	0.0471 (19)	0.052 (2)	0.0479 (17)	0.0216 (16)	0.0006 (14)	0.0005 (15)
C16	0.0480 (11)	0.1100 (18)	0.0564 (11)	0.0412 (12)	−0.0070 (9)	−0.0067 (11)
N4	0.0566 (12)	0.183 (3)	0.0910 (15)	0.0611 (15)	−0.0082 (11)	−0.0235 (16)

Geometric parameters (Å, º)

Fe1—N1^{i}	1.9688 (13)	C9—H9	0.9300
Fe1—N1^{ii}	1.9688 (13)	C10—H10	0.9300
Fe1—N1	1.9688 (13)	C11—C12^{iii}	1.422 (3)
Fe1—N2	1.9734 (13)	C11—C12^{iv}	1.422 (3)
Fe1—N2^{i}	1.9734 (13)	C11—C12	1.422 (3)
Fe1—N2^{ii}	1.9734 (13)	C11—C12^{v}	1.422 (3)
N1—C1	1.346 (2)	C11—C12^{vi}	1.422 (3)
N1—C5	1.355 (2)	C11—C12^{vii}	1.422 (3)
N2—C10	1.346 (2)	C12—C12^{iii}	1.423 (3)
N2—C6	1.354 (2)	C12—C12^{vii}	1.423 (3)
C1—C2	1.375 (2)	C12—C13	1.473 (3)
C1—H1	0.9300	C12—C13^{vii}	1.492 (3)
C2—C3	1.373 (3)	C13—N3	1.067 (2)
C2—H2	0.9300	C14—C15^{viii}	1.421 (3)
C3—C4	1.382 (3)	C14—C15^{ix}	1.421 (3)
C3—H3	0.9300	C14—C15	1.421 (3)
C4—C5	1.386 (2)	C14—C15^{x}	1.421 (3)
C4—H4	0.9300	C14—C15^{xi}	1.421 (3)
C5—C6	1.468 (2)	C14—C15^{xii}	1.422 (3)
C6—C7	1.384 (2)	C15—C15^{viii}	1.421 (3)
C7—C8	1.382 (3)	C15—C15^{xii}	1.422 (3)
C7—H7	0.9300	C15—C16	1.482 (4)
C8—C9	1.370 (3)	C15—C16^{xii}	1.482 (4)
C8—H8	0.9300	C16—N4	1.079 (3)
C9—C10	1.374 (2)		
N1^{i}—Fe1—N1^{ii}	96.74 (5)	C12^{iii}—C11—C12^{v}	60.040 (9)
N1^{i}—Fe1—N1	96.73 (5)	C12^{iv}—C11—C12^{v}	119.960 (9)
N1^{ii}—Fe1—N1	96.74 (5)	C12—C11—C12^{v}	119.960 (9)
N1^{i}—Fe1—N2	85.75 (5)	C12^{iii}—C11—C12^{vi}	119.964 (10)
N1^{ii}—Fe1—N2	177.07 (5)	C12^{iv}—C11—C12^{vi}	60.037 (9)
N1—Fe1—N2	81.40 (5)	C12—C11—C12^{vi}	180.0
N1^{i}—Fe1—N2^{i}	81.40 (5)	C12^{v}—C11—C12^{vi}	60.043 (9)
N1^{ii}—Fe1—N2^{i}	85.75 (5)	C12^{iii}—C11—C12^{vii}	119.962 (9)
N1—Fe1—N2^{i}	177.07 (5)	C12^{iv}—C11—C12^{vii}	60.037 (9)
N2—Fe1—N2^{i}	96.18 (5)	C12—C11—C12^{vii}	60.042 (9)

N1^{i}—Fe1—N2^{ii}	177.07 (5)	C12^{v}—C11—C12^{vii}	180.0
N1^{ii}—Fe1—N2^{ii}	81.40 (5)	C12^{vi}—C11—C12^{vii}	119.955 (9)
N1—Fe1—N2^{ii}	85.75 (5)	C11—C12—C12^{iii}	59.978 (4)
N2—Fe1—N2^{ii}	96.18 (5)	C11—C12—C12^{vii}	59.981 (5)
N2^{i}—Fe1—N2^{ii}	96.18 (5)	C12^{iii}—C12—C12^{vii}	119.84 (3)
C1—N1—C5	118.01 (14)	C11—C12—C13	117.8 (2)
C1—N1—Fe1	126.27 (11)	C12^{iii}—C12—C13	62.0 (2)
C5—N1—Fe1	115.13 (10)	C12^{vii}—C12—C13	162.7 (4)
C10—N2—C6	118.00 (14)	C11—C12—C13^{vii}	116.5 (2)
C10—N2—Fe1	126.53 (11)	C12^{iii}—C12—C13^{vii}	156.1 (4)
C6—N2—Fe1	115.18 (10)	C12^{vii}—C12—C13^{vii}	60.6 (2)
N1—C1—C2	122.79 (16)	C13—C12—C13^{vii}	125.6 (2)
N1—C1—H1	118.6	N3—C13—C12	151.6 (3)
C2—C1—H1	118.6	N3—C13—C12^{iii}	150.9 (2)
C3—C2—C1	119.18 (16)	C12—C13—C12^{iii}	57.34 (18)
C3—C2—H2	120.4	C15^{viii}—C14—C15^{ix}	180.0 (2)
C1—C2—H2	120.4	C15^{viii}—C14—C15	60.003 (4)
C2—C3—C4	119.04 (17)	C15^{ix}—C14—C15	119.996 (4)
C2—C3—H3	120.5	C15^{viii}—C14—C15^{x}	60.004 (3)
C4—C3—H3	120.5	C15^{ix}—C14—C15^{x}	119.997 (5)
C3—C4—C5	119.36 (17)	C15—C14—C15^{x}	119.997 (3)
C3—C4—H4	120.3	C15^{viii}—C14—C15^{xi}	120.000 (4)
C5—C4—H4	120.3	C15^{ix}—C14—C15^{xi}	60.001 (3)
N1—C5—C4	121.62 (15)	C15—C14—C15^{xi}	180.0
N1—C5—C6	113.92 (13)	C15^{x}—C14—C15^{xi}	60.006 (4)
C4—C5—C6	124.45 (15)	C15^{viii}—C14—C15^{xii}	119.998 (4)
N2—C6—C7	121.57 (15)	C15^{ix}—C14—C15^{xii}	60.001 (4)
N2—C6—C5	113.87 (13)	C15—C14—C15^{xii}	60.005 (4)
C7—C6—C5	124.56 (15)	C15^{x}—C14—C15^{xii}	180.0
C8—C7—C6	119.39 (18)	C15^{xi}—C14—C15^{xii}	119.991 (3)
C8—C7—H7	120.3	C14—C15—C15^{viii}	59.996 (2)
C6—C7—H7	120.3	C14—C15—C15^{xii}	59.999 (2)
C9—C8—C7	119.04 (17)	C15^{viii}—C15—C15^{xii}	119.984 (14)
C9—C8—H8	120.5	C14—C15—C16	116.8 (3)
C7—C8—H8	120.5	C15^{viii}—C15—C16	61.4 (3)
C8—C9—C10	119.21 (17)	C15^{xii}—C15—C16	159.4 (4)
C8—C9—H9	120.4	C14—C15—C16^{xii}	116.7 (3)
C10—C9—H9	120.4	C15^{viii}—C15—C16^{xii}	157.4 (4)
N2—C10—C9	122.77 (16)	C15^{xii}—C15—C16^{xii}	61.3 (3)
N2—C10—H10	118.6	C16—C15—C16^{xii}	126.5 (3)
C9—C10—H10	118.6	N4—C16—C15	151.5 (3)
C12^{iii}—C11—C12^{iv}	180.00 (17)	N4—C16—C15^{viii}	150.8 (3)
C12^{iii}—C11—C12	60.039 (9)	C15—C16—C15^{viii}	57.3 (2)
C12^{iv}—C11—C12	119.960 (9)		

C5—N1—C1—C2	−1.0 (2)	C12^{v}—C11—C12—C13	19.6 (4)
Fe1—N1—C1—C2	169.70 (14)	C12^{vii}—C11—C12—C13	−160.4 (4)
N1—C1—C2—C3	0.5 (3)	C12^{iii}—C11—C12—C13^{vii}	−153.1 (4)

C1—C2—C3—C4	0.4 (3)	C12^{iv}—C11—C12—C13^{vii}	26.9 (4)
C2—C3—C4—C5	−0.8 (3)	C12^{v}—C11—C12—C13^{vii}	−157.06 (12)
C1—N1—C5—C4	0.7 (2)	C12^{vii}—C11—C12—C13^{vii}	22.94 (12)
Fe1—N1—C5—C4	−171.07 (13)	C11—C12—C13—N3	153.0 (4)
C1—N1—C5—C6	179.30 (14)	C12^{iii}—C12—C13—N3	176.1 (5)
Fe1—N1—C5—C6	7.55 (17)	C12^{vii}—C12—C13—N3	75.2 (8)
C3—C4—C5—N1	0.2 (3)	C13^{vii}—C12—C13—N3	−30.7 (6)
C3—C4—C5—C6	−178.27 (17)	C11—C12—C13—C12^{iii}	−23.06 (8)
C10—N2—C6—C7	−0.9 (2)	C12^{vii}—C12—C13—C12^{iii}	−100.9 (7)
Fe1—N2—C6—C7	−175.08 (14)	C13^{vii}—C12—C13—C12^{iii}	153.2 (4)
C10—N2—C6—C5	178.43 (14)	C15^{ix}—C14—C15—C15^{viii}	180.0
Fe1—N2—C6—C5	4.22 (17)	C15^{x}—C14—C15—C15^{viii}	1.2 (5)
N1—C5—C6—N2	−7.7 (2)	C15^{xii}—C14—C15—C15^{viii}	−178.8 (5)
C4—C5—C6—N2	170.89 (15)	C15^{viii}—C14—C15—C15^{xii}	178.8 (5)
N1—C5—C6—C7	171.59 (16)	C15^{ix}—C14—C15—C15^{xii}	−1.2 (5)
C4—C5—C6—C7	−9.8 (3)	C15^{x}—C14—C15—C15^{xii}	180.0
N2—C6—C7—C8	1.2 (3)	C15^{viii}—C14—C15—C16	−24.35 (14)
C5—C6—C7—C8	−178.05 (18)	C15^{ix}—C14—C15—C16	155.65 (14)
C6—C7—C8—C9	−0.5 (3)	C15^{x}—C14—C15—C16	−23.2 (5)
C7—C8—C9—C10	−0.4 (3)	C15^{xii}—C14—C15—C16	156.8 (5)
C6—N2—C10—C9	−0.1 (3)	C15^{viii}—C14—C15—C16^{xii}	154.5 (5)
Fe1—N2—C10—C9	173.37 (14)	C15^{ix}—C14—C15—C16^{xii}	−25.5 (5)
C8—C9—C10—N2	0.8 (3)	C15^{x}—C14—C15—C16^{xii}	155.66 (14)
C12^{iv}—C11—C12—C12^{iii}	180.002 (1)	C15^{xii}—C14—C15—C16^{xii}	−24.34 (14)
C12^{v}—C11—C12—C12^{iii}	−4.0 (4)	C14—C15—C16—N4	−149.5 (4)
C12^{vii}—C11—C12—C12^{iii}	176.0 (4)	C15^{viii}—C15—C16—N4	−173.6 (5)
C12^{iii}—C11—C12—C12^{vii}	−176.0 (4)	C15^{xii}—C15—C16—N4	−74.0 (9)
C12^{iv}—C11—C12—C12^{vii}	4.0 (4)	C16^{xii}—C15—C16—N4	31.7 (7)
C12^{v}—C11—C12—C12^{vii}	180.0	C14—C15—C16—C15^{viii}	24.01 (10)
C12^{iii}—C11—C12—C13	23.55 (11)	C15^{xii}—C15—C16—C15^{viii}	99.5 (7)
C12^{iv}—C11—C12—C13	−156.45 (11)	C16^{xii}—C15—C16—C15^{viii}	−154.7 (5)

Symmetry codes: (i) $-y+2, x-y+1, z$; (ii) $-x+y+1, -x+2, z$; (iii) $x-y+2/3, x+1/3, -z+1/3$; (iv) $-x+y, -x+1, z$; (v) $-y+1, x-y+1, z$; (vi) $-x+2/3, -y+4/3, -z+1/3$; (vii) $y-1/3, -x+y+1/3, -z+1/3$; (viii) $y+1/3, -x+y+2/3, -z+2/3$; (ix) $-y+1, x-y, z$; (x) $-x+y+1, -x+1, z$; (xi) $-x+4/3, -y+2/3, -z+2/3$; (xii) $x-y+1/3, x-1/3, -z+2/3$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1^{ii}	0.93	2.61	3.121 (2)	115
C10—H10···N2^{i}	0.93	2.60	3.116 (2)	115
C4—H4···N3^{v}	0.93	2.45	3.333 (3)	159
C8—H8···N3^{iii}	0.93	2.68	3.476 (3)	144
C3—H3···N4^{v}	0.93	2.65	3.244 (3)	122
C10—H10···N4^{xiii}	0.93	2.68	3.437 (3)	139

Symmetry codes: (i) $-y+2, x-y+1, z$; (ii) $-x+y+1, -x+2, z$; (iii) $x-y+2/3, x+1/3, -z+1/3$; (v) $-y+1, x-y+1, z$; (xiii) $-y+4/3, x-y+2/3, z-1/3$.