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## Dichloro[*N,N,N',N'*-tetrakis(2-pyridylmethyl)benzene-1,4-diamine]iron(II)

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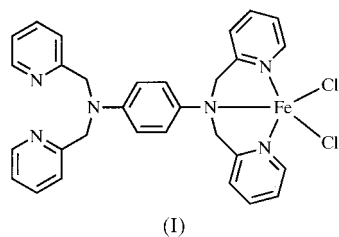
Received 25 October 2000

Accepted 9 November 2000

In the title complex, [FeCl<sub>2</sub>(C<sub>30</sub>H<sub>28</sub>N<sub>6</sub>)], the Fe atom is five-coordinated by two terminal chloride ligands and one end of the bis-tridentate ligand. The complexes display intermolecular C—H···π, π-stacking and C—H···X (X = N, Cl) interactions.

### Comment

The ligand *N,N,N',N'*-tetrakis(2-pyridylmethyl)benzene-1,4-diamine (1,4-tpbd) is capable of forming both mono- and dinuclear complexes (Buchen *et al.*, 1997; Hazell *et al.*, 1998). Also, the coordination of octahedral metal ions as connectors between the tridentate bis(2-pyridylmethyl)amine ends of two 1,4-tpbd ligands should make possible the formation of one-dimensional coordination polymers. The title complex, (I), was obtained in the course of our efforts to access an iron(II)-containing polymer. Such a polymeric complex may be particularly interesting due to the similarity of the N<sub>6</sub> environment to well known mononuclear spin-crossover systems (Gütlich *et al.*, 1994). The reaction of several iron(II) salts with 1,4-tpbd has led to the precipitation of yellow powders which have shown a 1:1 ligand–metal stoichiometry by elemental analysis, commensurable with either mononuclear or coordination polymeric structures (dinuclear could be excluded on this basis). The title compound, (I), was obtained as a yellow crystalline material from the reaction of iron(II) chloride with

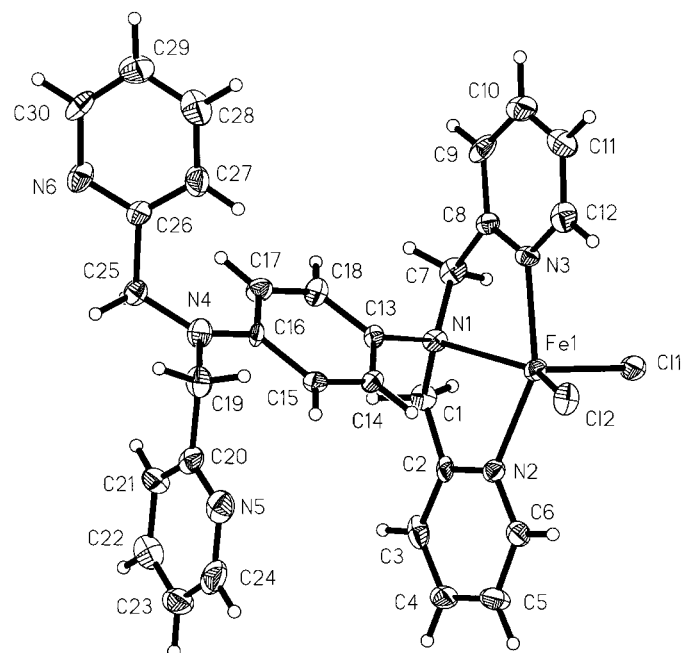


1,4-tpbd and the structure reported here shows it to be monomeric. The cell parameters and space group are similar to the Zn analogue (Hazell *et al.*, 1998), however, the packing

of the complexes in the two structures differs to some extent, and thus the two structures are not strictly isostructural.

A search of the Cambridge Structural Database (update 5.19, April 2000; Allen & Kennard, 1993) reveals that (I) is only the third example of pentacoordinated iron(II) with an N<sub>3</sub>Cl<sub>2</sub> ligand set (Small *et al.*, 1998; Britovsek *et al.*, 1998; Hemmert *et al.*, 1999). The geometry around the Fe atom (Table 1) is best described as being closer to square pyramidal (with C11 at the apex) than trigonal bipyramidal, although the geometry is more distorted from square pyramidal compared with the two other pentacoordinated iron(II) complexes with N<sub>3</sub>Cl<sub>2</sub> coordination spheres. The sum of the C—N—C angles around the uncoordinated phenylenediamine N atom is 359.1 (9)°, and C16—N4 is only 1.386 (9) Å, indicating a π delocalization of this amine N atom lone pair with the aromatic system. In contrast, the corresponding values for the coordinated amine N atom are 335.8 (10)° and 1.475 (8) Å, respectively.

The H-shaped complexes are interdigitated and display C—H···π interactions between a CH group of a coordinated pyridyl ring of one complex and the benzene ring of another [closest contact: C4···C14<sup>iv</sup> = 3.620 (9) Å, H4A···C14<sup>iv</sup> = 2.69 Å, C4—H4A···C14<sup>iv</sup> = 165°; symmetry code: (iv) x + 1, y, z]. This pyridyl ring also engages in π-stacking interactions with a coordinated pyridyl of this second complex [closest non-hydrogen interaction: C5···C12<sup>iv</sup> = 3.34 (1) Å], which in turn engages in a π-stacking interaction with an uncoordinated pyridyl ring of a third complex [closest non-hydrogen interaction: C11···C24<sup>v</sup> = 3.28 (1) Å; symmetry code: (v) x, y, z + 1]. There are also a number of close C—H···X intermolecular contacts between both aromatic and aliphatic H atoms and the uncoordinated pyridyl N atoms and the chloride ligands which connect the complexes (Table 2).



**Figure 1**

A view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

## Experimental

The title compound was prepared from the 1:1 reaction of anhydrous  $\text{FeCl}_2$  and 1,4-tpbd in acetonitrile under an inert atmosphere (Hazell *et al.*, 1998). Yellow single crystals suitable for analysis were obtained directly from the reaction mixture.

### Crystal data

$[\text{FeCl}_2(\text{C}_{30}\text{H}_{28}\text{N}_6)]$	$D_x = 1.457 \text{ Mg m}^{-3}$
$M_r = 599.33$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 11554 reflections
$a = 8.4470 (6) \text{ \AA}$	$\theta = 3.16\text{--}28.26^\circ$
$b = 12.9100 (12) \text{ \AA}$	$\mu = 0.780 \text{ mm}^{-1}$
$c = 12.9850 (13) \text{ \AA}$	$T = 123 (2) \text{ K}$
$\beta = 105.270 (6)^\circ$	Irregular block, yellow
$V = 1366.0 (2) \text{ \AA}^3$	$0.125 \times 0.125 \times 0.075 \text{ mm}$
$Z = 2$	

### Data collection

Nonius KappaCCD diffractometer	$R_{\text{int}} = 0.110$
$\varphi$ and $\omega$ scans	$\theta_{\text{max}} = 28.26^\circ$
11 514 measured reflections	$h = -9 \rightarrow 11$
3479 independent reflections (plus 1813 Friedel-related reflections)	$k = -12 \rightarrow 17$
3608 reflections with $I > 2\sigma(I)$	$l = -17 \rightarrow 17$
	Intensity decay: $<1\%$

### Refinement

Refinement on $F^2$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.080$	$\Delta\rho_{\text{max}} = 1.03 \text{ e \AA}^{-3}$
$wR(F^2) = 0.156$	$\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$
$S = 1.061$	Absolute structure: Flack (1983)
5292 reflections	Flack parameter = 0.01 (3)
352 parameters	
H-atom parameters constrained	
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 3.2934P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

The support of the Danish Natural Science Research Council (CJM) and receipt of an ARC Postdoctoral Fellowship (SRB) is gratefully acknowledged.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Fe1—N3	2.141 (5)	Fe1—Cl2	2.321 (2)
Fe1—N2	2.152 (5)	Fe1—Cl1	2.329 (2)
Fe1—N1	2.251 (6)		
N3—Fe1—N2	151.4 (2)	N1—Fe1—Cl2	136.3 (2)
N3—Fe1—N1	75.7 (2)	N3—Fe1—Cl1	95.8 (2)
N2—Fe1—N1	75.8 (2)	N2—Fe1—Cl1	96.3 (2)
N3—Fe1—Cl2	98.8 (2)	N1—Fe1—Cl1	110.4 (2)
N2—Fe1—Cl2	100.0 (2)	Cl2—Fe1—Cl1	113.24 (8)

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C11—H11A $\cdots$ Cl1 <sup>i</sup>	0.95	2.76	3.556 (7)	142
C23—H23A $\cdots$ Cl1 <sup>ii</sup>	0.95	2.80	3.666 (8)	152
C25—H25A $\cdots$ Cl2 <sup>iii</sup>	0.99	2.75	3.730 (8)	169
C17—H17A $\cdots$ N5 <sup>iii</sup>	0.95	2.55	3.42 (1)	153

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

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1490). Services for accessing these data are described at the back of the journal.

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## supporting information

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### Computing details

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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#### Crystal data

[FeCl<sub>2</sub>(C<sub>30</sub>H<sub>28</sub>N<sub>6</sub>)]

$M_r = 599.33$

Monoclinic,  $P2_1$

$a = 8.4470$  (6) Å

$b = 12.9100$  (12) Å

$c = 12.9850$  (13) Å

$\beta = 105.270$  (6)°

$V = 1366.0$  (2) Å<sup>3</sup>

$Z = 2$

$F(000) = 620$

$D_x = 1.457$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 11554 reflections

$\theta = 3.2$ – $28.3$ °

$\mu = 0.78$  mm<sup>-1</sup>

$T = 123$  K

Irregular block, yellow

$0.13 \times 0.13 \times 0.08$  mm

#### Data collection

Nonius KappaCCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 9 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

11514 measured reflections

5292 independent reflections

3608 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.110$

$\theta_{\text{max}} = 28.3$ °,  $\theta_{\text{min}} = 3.2$ °

$h = -9 \rightarrow 11$

$k = -12 \rightarrow 17$

$l = -17 \rightarrow 17$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.080$

$wR(F^2) = 0.156$

$S = 1.06$

5292 reflections

352 parameters

1 restraint

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 3.2934P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.03$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.66$  e Å<sup>-3</sup>

Absolute structure: Flack (1983), 1813 Friedel  
pairs

Absolute structure parameter: 0.01 (3)

*Special details*

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.40540 (11)	0.54750 (8)	0.43159 (7)	0.0200 (3)
Cl1	0.58024 (19)	0.53142 (16)	0.60247 (13)	0.0278 (5)
Cl2	0.2987 (2)	0.39034 (13)	0.35798 (15)	0.0277 (4)
N1	0.3807 (6)	0.7149 (4)	0.3814 (5)	0.0171 (12)
C1	0.5486 (7)	0.7511 (5)	0.3777 (6)	0.0204 (16)
H1A	0.5379	0.8125	0.3306	0.024*
H1B	0.6126	0.7716	0.4501	0.024*
C2	0.6369 (8)	0.6666 (5)	0.3365 (5)	0.0188 (15)
C3	0.7674 (8)	0.6892 (6)	0.2918 (6)	0.0283 (19)
H3A	0.7951	0.7590	0.2812	0.034*
C4	0.8546 (9)	0.6088 (7)	0.2637 (6)	0.0283 (19)
H4A	0.9445	0.6226	0.2345	0.034*
C5	0.8103 (9)	0.5079 (7)	0.2782 (6)	0.031 (2)
H5A	0.8681	0.4511	0.2588	0.038*
C6	0.6779 (8)	0.4916 (6)	0.3221 (5)	0.0236 (17)
H6A	0.6460	0.4226	0.3320	0.028*
N2	0.5948 (6)	0.5697 (4)	0.3507 (4)	0.0190 (14)
C7	0.3294 (8)	0.7655 (6)	0.4698 (6)	0.0230 (17)
H7A	0.2912	0.8368	0.4489	0.028*
H7B	0.4238	0.7696	0.5338	0.028*
C8	0.1926 (8)	0.7036 (5)	0.4951 (5)	0.0187 (15)
C9	0.0722 (8)	0.7490 (6)	0.5365 (6)	0.0272 (18)
H9A	0.0671	0.8220	0.5439	0.033*
C10	-0.0408 (9)	0.6843 (7)	0.5668 (6)	0.0308 (19)
H10A	-0.1228	0.7128	0.5963	0.037*
C11	-0.0318 (9)	0.5806 (7)	0.5536 (6)	0.034 (2)
H11A	-0.1076	0.5354	0.5734	0.041*
C12	0.0892 (7)	0.5416 (8)	0.5110 (5)	0.0283 (16)
H12A	0.0948	0.4689	0.5017	0.034*
N3	0.1985 (6)	0.6018 (4)	0.4822 (4)	0.0187 (13)
C13	0.2610 (7)	0.7263 (5)	0.2764 (5)	0.0162 (14)
C14	0.2437 (8)	0.6473 (5)	0.2013 (6)	0.0185 (15)
H14A	0.3061	0.5857	0.2200	0.022*
C15	0.1392 (8)	0.6559 (5)	0.1011 (6)	0.0199 (15)
H15A	0.1327	0.6014	0.0510	0.024*

C16	0.0399 (9)	0.7462 (5)	0.0715 (6)	0.0202 (16)
C17	0.0588 (9)	0.8243 (5)	0.1481 (6)	0.0235 (17)
H17A	-0.0053	0.8855	0.1315	0.028*
C18	0.1684 (8)	0.8148 (5)	0.2474 (6)	0.0220 (16)
H18A	0.1804	0.8704	0.2967	0.026*
N4	-0.0702 (7)	0.7538 (5)	-0.0284 (5)	0.0262 (15)
C19	-0.0808 (9)	0.6716 (6)	-0.1053 (6)	0.0290 (18)
H19A	-0.1759	0.6852	-0.1670	0.035*
H19B	-0.1020	0.6056	-0.0724	0.035*
C20	0.0722 (9)	0.6585 (6)	-0.1459 (6)	0.0252 (17)
C21	0.1731 (9)	0.7411 (6)	-0.1506 (6)	0.0323 (19)
H21A	0.1505	0.8077	-0.1270	0.039*
C22	0.3072 (10)	0.7255 (7)	-0.1902 (6)	0.037 (2)
H22A	0.3772	0.7817	-0.1954	0.044*
C23	0.3383 (10)	0.6290 (7)	-0.2217 (6)	0.039 (2)
H23A	0.4307	0.6164	-0.2486	0.047*
C24	0.2328 (10)	0.5495 (9)	-0.2136 (5)	0.0412 (19)
H24A	0.2551	0.4820	-0.2352	0.049*
N5	0.0991 (7)	0.5636 (5)	-0.1762 (5)	0.0327 (16)
C25	-0.1533 (9)	0.8509 (6)	-0.0635 (6)	0.0273 (18)
H25A	-0.1846	0.8522	-0.1425	0.033*
H25B	-0.0748	0.9082	-0.0385	0.033*
C26	-0.3064 (8)	0.8711 (6)	-0.0252 (5)	0.0227 (17)
C27	-0.3662 (9)	0.8030 (7)	0.0356 (6)	0.0312 (19)
H27A	-0.3125	0.7386	0.0557	0.037*
C28	-0.5053 (9)	0.8276 (7)	0.0680 (7)	0.037 (2)
H28A	-0.5493	0.7805	0.1094	0.044*
C29	-0.5775 (9)	0.9217 (7)	0.0387 (7)	0.036 (2)
H29A	-0.6706	0.9426	0.0615	0.043*
C30	-0.5126 (9)	0.9849 (6)	-0.0242 (6)	0.0317 (19)
H30A	-0.5669	1.0485	-0.0473	0.038*
N6	-0.3754 (7)	0.9623 (5)	-0.0555 (5)	0.0284 (15)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Fe1	0.0167 (5)	0.0202 (5)	0.0235 (5)	0.0023 (5)	0.0059 (4)	0.0021 (5)
C11	0.0207 (8)	0.0401 (13)	0.0216 (9)	0.0080 (9)	0.0037 (7)	0.0032 (9)
C12	0.0295 (10)	0.0221 (10)	0.0276 (11)	-0.0037 (8)	0.0005 (8)	0.0008 (8)
N1	0.007 (2)	0.019 (3)	0.024 (3)	-0.006 (2)	0.002 (2)	-0.001 (3)
C1	0.012 (3)	0.021 (4)	0.026 (4)	-0.008 (3)	0.002 (3)	-0.001 (3)
C2	0.012 (3)	0.026 (4)	0.015 (4)	0.001 (3)	-0.003 (3)	0.008 (3)
C3	0.017 (4)	0.040 (5)	0.024 (4)	-0.007 (4)	-0.003 (3)	0.013 (4)
C4	0.014 (4)	0.046 (5)	0.025 (4)	0.005 (4)	0.006 (3)	0.005 (4)
C5	0.029 (4)	0.043 (5)	0.027 (4)	0.006 (4)	0.015 (4)	-0.001 (4)
C6	0.017 (4)	0.033 (4)	0.019 (4)	0.000 (3)	0.003 (3)	0.004 (3)
N2	0.017 (3)	0.020 (4)	0.019 (3)	0.002 (2)	0.004 (2)	0.001 (2)
C7	0.017 (3)	0.026 (4)	0.021 (4)	-0.002 (3)	-0.004 (3)	-0.006 (3)

C8	0.016 (3)	0.023 (4)	0.016 (4)	0.003 (3)	0.001 (3)	-0.002 (3)
C9	0.022 (4)	0.030 (5)	0.023 (4)	0.011 (3)	-0.006 (3)	-0.004 (3)
C10	0.014 (4)	0.051 (6)	0.025 (4)	0.006 (4)	0.000 (3)	-0.002 (4)
C11	0.017 (3)	0.062 (7)	0.020 (4)	0.001 (4)	0.001 (3)	0.003 (4)
C12	0.020 (3)	0.034 (4)	0.027 (4)	-0.003 (4)	-0.001 (3)	0.003 (4)
N3	0.012 (3)	0.028 (4)	0.016 (3)	0.000 (3)	0.002 (2)	-0.002 (3)
C13	0.011 (3)	0.020 (4)	0.016 (4)	-0.002 (3)	0.000 (3)	0.003 (3)
C14	0.012 (3)	0.015 (4)	0.029 (4)	-0.001 (3)	0.007 (3)	0.005 (3)
C15	0.017 (3)	0.022 (4)	0.022 (4)	0.001 (3)	0.008 (3)	0.000 (3)
C16	0.018 (3)	0.022 (4)	0.020 (4)	0.007 (3)	0.004 (3)	0.012 (3)
C17	0.026 (4)	0.021 (4)	0.024 (4)	0.003 (3)	0.007 (3)	-0.004 (3)
C18	0.023 (4)	0.016 (4)	0.024 (4)	-0.003 (3)	0.001 (3)	0.000 (3)
N4	0.024 (3)	0.030 (4)	0.021 (3)	0.000 (3)	-0.001 (3)	0.001 (3)
C19	0.026 (4)	0.040 (5)	0.015 (4)	0.001 (4)	-0.005 (3)	0.000 (4)
C20	0.021 (4)	0.031 (4)	0.018 (4)	0.006 (3)	-0.004 (3)	-0.001 (3)
C21	0.033 (4)	0.043 (5)	0.024 (4)	0.007 (4)	0.013 (4)	0.005 (4)
C22	0.039 (5)	0.041 (5)	0.031 (5)	-0.005 (4)	0.009 (4)	0.003 (4)
C23	0.028 (4)	0.065 (7)	0.024 (5)	0.012 (5)	0.008 (4)	0.004 (4)
C24	0.047 (5)	0.045 (5)	0.025 (4)	0.021 (6)	-0.001 (4)	0.006 (5)
N5	0.037 (3)	0.034 (4)	0.023 (3)	0.002 (3)	0.000 (3)	-0.003 (3)
C25	0.020 (4)	0.036 (5)	0.025 (4)	0.008 (4)	0.004 (3)	0.009 (4)
C26	0.010 (3)	0.036 (5)	0.018 (4)	0.004 (3)	-0.004 (3)	0.001 (3)
C27	0.026 (4)	0.039 (5)	0.027 (5)	0.003 (4)	0.003 (4)	0.011 (4)
C28	0.024 (4)	0.049 (6)	0.035 (5)	-0.013 (4)	0.003 (4)	0.006 (4)
C29	0.019 (4)	0.043 (5)	0.047 (5)	-0.004 (4)	0.011 (4)	-0.001 (4)
C30	0.022 (4)	0.029 (4)	0.039 (5)	0.012 (3)	-0.002 (4)	0.000 (4)
N6	0.017 (3)	0.029 (4)	0.034 (4)	0.001 (3)	-0.002 (3)	0.005 (3)

*Geometric parameters (Å, °)*

Fe1—N3	2.141 (5)	C13—C14	1.391 (9)
Fe1—N2	2.152 (5)	C14—C15	1.371 (9)
Fe1—N1	2.251 (6)	C15—C16	1.428 (9)
Fe1—C12	2.321 (2)	C16—N4	1.386 (9)
Fe1—C11	2.329 (2)	C16—C17	1.396 (9)
N1—C13	1.475 (8)	C17—C18	1.381 (9)
N1—C7	1.481 (9)	N4—C19	1.444 (10)
N1—C1	1.506 (8)	N4—C25	1.450 (9)
C1—C2	1.498 (9)	C19—C20	1.529 (10)
C2—N2	1.326 (8)	C20—N5	1.325 (10)
C2—C3	1.405 (9)	C20—C21	1.376 (11)
C3—C4	1.377 (11)	C21—C22	1.376 (11)
C4—C5	1.383 (10)	C22—C23	1.359 (12)
C5—C6	1.399 (10)	C23—C24	1.380 (13)
C6—N2	1.335 (8)	C24—N5	1.354 (9)
C7—C8	1.511 (9)	C25—C26	1.526 (10)
C8—N3	1.328 (8)	C26—N6	1.327 (9)
C8—C9	1.398 (9)	C26—C27	1.365 (10)

C9—C10	1.400 (11)	C27—C28	1.385 (11)
C10—C11	1.355 (11)	C28—C29	1.367 (11)
C11—C12	1.379 (10)	C29—C30	1.367 (11)
C12—N3	1.334 (9)	C30—N6	1.357 (9)
C13—C18	1.380 (9)		
N3—Fe1—N2	151.4 (2)	C8—N3—C12	119.3 (6)
N3—Fe1—N1	75.7 (2)	C8—N3—Fe1	115.1 (4)
N2—Fe1—N1	75.8 (2)	C12—N3—Fe1	125.2 (5)
N3—Fe1—C12	98.8 (2)	C18—C13—C14	117.9 (6)
N2—Fe1—C12	100.0 (2)	C18—C13—N1	122.5 (6)
N1—Fe1—C12	136.3 (2)	C14—C13—N1	119.6 (6)
N3—Fe1—C11	95.8 (2)	C15—C14—C13	121.9 (6)
N2—Fe1—C11	96.3 (2)	C14—C15—C16	120.4 (7)
N1—Fe1—C11	110.4 (2)	N4—C16—C17	122.5 (6)
C12—Fe1—C11	113.24 (8)	N4—C16—C15	120.7 (6)
C13—N1—C7	113.7 (5)	C17—C16—C15	116.7 (7)
C13—N1—C1	111.2 (5)	C18—C17—C16	121.5 (6)
C7—N1—C1	110.9 (5)	C13—C18—C17	121.5 (6)
C13—N1—Fe1	110.6 (4)	C16—N4—C19	120.0 (6)
C7—N1—Fe1	102.9 (4)	C16—N4—C25	120.4 (6)
C1—N1—Fe1	107.0 (4)	C19—N4—C25	118.7 (6)
C2—C1—N1	110.3 (5)	N4—C19—C20	114.5 (6)
N2—C2—C3	121.5 (7)	N5—C20—C21	123.1 (7)
N2—C2—C1	117.4 (6)	N5—C20—C19	115.5 (7)
C3—C2—C1	120.9 (6)	C21—C20—C19	121.3 (7)
C4—C3—C2	119.0 (7)	C20—C21—C22	119.0 (8)
C3—C4—C5	119.5 (6)	C23—C22—C21	119.3 (8)
C4—C5—C6	118.1 (7)	C22—C23—C24	118.6 (8)
N2—C6—C5	122.4 (7)	N5—C24—C23	122.9 (9)
C2—N2—C6	119.5 (6)	C20—N5—C24	117.1 (8)
C2—N2—Fe1	117.0 (4)	N4—C25—C26	115.3 (6)
C6—N2—Fe1	123.2 (4)	N6—C26—C27	122.9 (6)
N1—C7—C8	109.4 (5)	N6—C26—C25	113.5 (6)
N3—C8—C9	121.2 (6)	C27—C26—C25	123.6 (7)
N3—C8—C7	116.0 (5)	C26—C27—C28	120.0 (8)
C9—C8—C7	122.6 (6)	C29—C28—C27	118.1 (8)
C8—C9—C10	118.5 (7)	C28—C29—C30	118.5 (7)
C11—C10—C9	119.3 (7)	N6—C30—C29	124.0 (7)
C10—C11—C12	118.9 (8)	C26—N6—C30	116.4 (6)
N3—C12—C11	122.8 (9)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11A $\cdots$ C11 <sup>i</sup>	0.95	2.76	3.556 (7)	142
C23—H23A $\cdots$ C11 <sup>ii</sup>	0.95	2.80	3.666 (8)	152



C25—H25A $\cdots$ C12 <sup>iii</sup>	0.99	2.75	3.730 (8)	169
C17—H17A $\cdots$ N5 <sup>iii</sup>	0.95	2.55	3.42 (1)	153

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