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(2,2′-Bipyridine-κ^2N,N')(4′-ferrocenyl-2,2′:6′,2″-terpyridine-κ^3N,N',N'')-copper(II) bis(tetrafluoridoborate)

Si-Ping Tang* and Dai-Zhi Kuang

Department of Chemistry and Materials Science, Hengyang Normal University, Hengyang, Hunan 421008, People's Republic of China
Correspondence e-mail: sptang88@163.com

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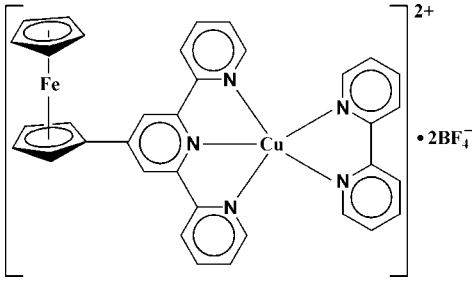
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.059; wR factor = 0.163; data-to-parameter ratio = 16.3.

In the title complex, $[CuFe(C_5H_5)(C_{20}H_{14}N_3)(C_{10}H_8N_2)](BF_4)_2$, the Cu^{II} atom is five-coordinated by a tridentate chelating 4′-ferrocenyl-2,2′:6′,2″-terpyridine (fctpy) ligand and a bidentate chelating 2,2′-bipyridine (bpy) ligand. The coordination polyhedron is distorted square-pyramidal with an N atom from the bipyridine ligand in the apical position at a Cu—N distance of 2.195 (3) Å. In the crystal structure, tetrafluoridoborate counter-ions are involved as acceptors in intermolecular C—H···F hydrogen-bonding interactions with both the bipyridyl and terpyridyl ligands, resulting in a three-dimensional supramolecular structure.

Related literature

For general background, see: Andres & Schubert (2004); Barigelletti & Flamigni (2000); Licini & Williams (1999). For a functionalized terpyridine complex, see: Hofmeier & Schubert (2004). For 4′-ferrocenyl-2,2′:6′,2″-terpyridine–metal complexes, see: Aguado *et al.* (2005); Constable *et al.* (1994); Farlow *et al.* (1993).



Experimental

Crystal data

$[CuFe(C_5H_5)(C_{20}H_{14}N_3)(C_{10}H_8N_2)](BF_4)_2$
M_r = 810.63
Monoclinic, $P2_1/n$
a = 14.0780 (8) Å
b = 14.2074 (8) Å
c = 16.9442 (10) Å
β = 95.488 (1)°
V = 3373.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.804, T_{max} = 0.895
20780 measured reflections
7656 independent reflections
5667 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.163
S = 1.05
7656 reflections
469 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F4^{i}	0.93	2.51	3.306 (5)	143
C4—H4···F8^{ii}	0.93	2.40	3.176 (6)	141
C17—H17···F7^{ii}	0.93	2.39	3.296 (5)	165
C13—H13···F3^{iii}	0.93	2.54	3.140 (6)	123
C34—H34···F2	0.93	2.48	3.274 (6)	144
C35—H35···F1	0.93	2.37	3.208 (6)	149

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

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: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

We thank Hengyang Normal University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2416).

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supplementary materials

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(2,2'-Bipyridine-κ^2N,N')(4'-ferrocenyl-2,2':6',2''-terpyridine-κ^3N,N',N'')copper(II) bis(tetrafluoridoborate)

S.-P. Tang and D.-Z. Kuang

Comment

The chemistry of 2,2':6',2''-terpyridine (tpy) ligand has been the subject of numerous studies because of its good chelating ability towards transition metal ions, and some of its complexes are promising materials for potential applications as luminescent devices (Andres & Schubert, 2004; Barigelletti & Flamigni, 2000; Licini & Williams, 1999). Especially, the central pyridyl ring can be easily functionalized to attain different aims, and much work has been done on functionalized terpyridine complexes (Hofmeier & and Schubert, 2004). For example, several studies have been carried out on the structure and electrochemical properties of 4'-ferrocenyl-2,2':6',2''-terpyridine (fctpy) and its Au^{I}, Ru^{II}, Co^{II} and Fe^{II} complexes (Aguado *et al.*, 2005; Constable *et al.*, 1994; Farlow *et al.*, 1993). In this work, we represent a new mixed-ligand complex, incorporating fctpy and 2,2'-bipyridine (bpy) ligands.

In the title complex, (I), Fig. 1, the Cu^{II} atom is five-coordinated by three N atoms from the fctpy ligand and two N atoms from the bpy, ligand displaying a distorted square pyramidal geometry. The apex of the pyramid is occupied by the N5 from the bpy ligand with a Cu1—N5 distance of 2.195 (3) Å, which is somewhat longer than those in the basal plane [Cu—N distances in the range 1.928 (3)–2.062 (3) Å]. The angles subtended at Cu(1) by the tridentate terpyridyl ligand are 79.52 (12) and 80.08 (12) ° respectively. The two cyclopentadienyl rings of the ferrocenyl group are almost eclipsed and the dihedral angle between the two rings is 5.1 (2) °.

In the crystal structure, tetrafluoridoborate counterions are involved as acceptors in intermolecular C—H···F hydrogen-bonding interactions with both the bipyridyl and terpyridyl ligands, resulting a three-dimensional supramolecular structure, Table 1.

Experimental

The ligand fctpy was synthesized according to the reported procedure (Farlow *et al.*, 1993). A solution of copper fluoroborate hydrate (69.8 mg, 0.2 mmol), fctpy (82.5 mg, 0.2 mmol) and 2,2'-bipyridine (32.1 g, 0.2 mmol) in methanol (15 ml) was stirred for 4 h. The product was filtered off and dried. The precipitate were recrystallized from acetonitrile (10 ml) to give black block-shaped crystals of the title complex after one week. Yield: 105 mg (65%).

Refinement

The carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and refined as riding, with U(H) = 1.2U_{eq}(C).

Figures

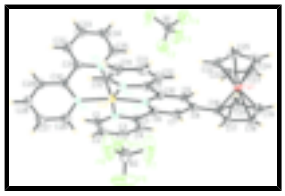


Fig. 1. The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level, and H atoms as spheres of arbitrary radius.

(2,2'-Bipyridine-κ^2*N*,*N*')(4'-ferrocenyl-2,2':6',2''-terpyridine- κ^3*N*,*N*',*N*'')copper(II) bis(tetrafluoridoborate)

Crystal data

$[CuFe(C_5H_5)(C_{20}H_{14}N_3)(C_{10}H_8N_2)](BF_4)_2$	F_{000} = 1636
M_r = 810.63	D_x = 1.596 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3768 reflections
a = 14.0780 (8) Å	θ = 2.4–23.2º
b = 14.2074 (8) Å	μ = 1.14 mm^{-1}
c = 16.9442 (10) Å	T = 293 (2) K
β = 95.488 (1)º	Block, orange
V = 3373.5 (3) Å^3	0.20 × 0.18 × 0.10 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	7656 independent reflections
Radiation source: fine-focus sealed tube	5667 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −18→12
T_{min} = 0.804, T_{max} = 0.895	k = −18→18
20780 measured reflections	l = −19→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.163	$w = 1/[\sigma^2(F_o^2) + (0.0922P)^2 + 0.8536P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$

7656 reflections	$\Delta\rho_{max} = 0.89$ e Å^{-3}
469 parameters	$\Delta\rho_{min} = -0.74$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	−0.10157 (3)	0.23820 (3)	0.12009 (3)	0.03846 (15)
Fe1	0.38524 (4)	0.01582 (4)	0.12953 (3)	0.03927 (17)
N1	−0.0949 (2)	0.2164 (2)	0.00040 (18)	0.0405 (7)
N2	0.0094 (2)	0.1584 (2)	0.12231 (16)	0.0364 (6)
N3	−0.0788 (2)	0.2132 (2)	0.23883 (18)	0.0400 (7)
N4	−0.2275 (2)	0.3013 (2)	0.11664 (18)	0.0402 (7)
N5	−0.0599 (2)	0.3868 (2)	0.11526 (18)	0.0398 (7)
C1	−0.1545 (3)	0.2491 (3)	−0.0600 (2)	0.0467 (9)
H1	−0.2070	0.2846	−0.0487	0.056*
C2	−0.1409 (3)	0.2319 (3)	−0.1378 (3)	0.0554 (11)
H2	−0.1840	0.2548	−0.1783	0.066*
C3	−0.0634 (4)	0.1809 (3)	−0.1554 (2)	0.0555 (11)
H3	−0.0532	0.1684	−0.2078	0.067*
C4	−0.0001 (3)	0.1480 (3)	−0.0937 (2)	0.0498 (10)
H4	0.0539	0.1143	−0.1041	0.060*
C5	−0.0186 (3)	0.1662 (2)	−0.0169 (2)	0.0388 (8)
C6	0.0418 (3)	0.1303 (2)	0.0539 (2)	0.0388 (8)
C7	0.1199 (3)	0.0721 (2)	0.0536 (2)	0.0390 (8)
H7	0.1423	0.0543	0.0060	0.047*
C8	0.1653 (3)	0.0398 (2)	0.1259 (2)	0.0382 (8)
C9	0.1277 (3)	0.0674 (2)	0.1957 (2)	0.0387 (8)
H9	0.1556	0.0463	0.2445	0.046*
C10	0.0495 (3)	0.1260 (2)	0.1922 (2)	0.0363 (8)
C11	−0.0021 (3)	0.1583 (2)	0.2599 (2)	0.0382 (8)
C12	0.0236 (3)	0.1346 (3)	0.3378 (2)	0.0456 (9)
H12	0.0773	0.0978	0.3514	0.055*
C13	−0.0319 (3)	0.1663 (3)	0.3955 (2)	0.0553 (11)
H13	−0.0165	0.1504	0.4484	0.066*

C14	−0.1094 (3)	0.2212 (3)	0.3739 (3)	0.0570 (11)
H14	−0.1475	0.2431	0.4120	0.068*
C15	−0.1309 (3)	0.2440 (3)	0.2954 (3)	0.0513 (10)
H15	−0.1835	0.2821	0.2812	0.062*
C16	0.2469 (3)	−0.0242 (2)	0.1279 (2)	0.0388 (8)
C17	0.2887 (3)	−0.0628 (2)	0.0609 (2)	0.0433 (8)
H17	0.2680	−0.0521	0.0079	0.052*
C18	0.3666 (3)	−0.1198 (3)	0.0895 (3)	0.0477 (9)
H18	0.4058	−0.1532	0.0583	0.057*
C19	0.3753 (3)	−0.1178 (3)	0.1735 (3)	0.0521 (10)
H19	0.4215	−0.1488	0.2069	0.062*
C20	0.3006 (3)	−0.0597 (3)	0.1976 (2)	0.0448 (9)
H20	0.2889	−0.0470	0.2497	0.054*
C21	0.3866 (4)	0.1578 (3)	0.1202 (4)	0.0723 (14)
H21	0.3331	0.1965	0.1139	0.087*
C22	0.4337 (4)	0.1174 (3)	0.0592 (3)	0.0668 (12)
H22	0.4166	0.1242	0.0051	0.080*
C23	0.5110 (3)	0.0651 (3)	0.0941 (3)	0.0603 (11)
H23	0.5546	0.0316	0.0672	0.072*
C24	0.5112 (3)	0.0721 (3)	0.1762 (3)	0.0637 (12)
H24	0.5546	0.0436	0.2136	0.076*
C25	0.4350 (4)	0.1291 (3)	0.1926 (3)	0.0695 (13)
H25	0.4189	0.1454	0.2428	0.083*
C26	−0.3100 (3)	0.2553 (3)	0.1214 (3)	0.0530 (10)
H26	−0.3088	0.1902	0.1272	0.064*
C27	−0.3961 (3)	0.3010 (3)	0.1181 (3)	0.0605 (12)
H27	−0.4522	0.2674	0.1219	0.073*
C28	−0.3986 (3)	0.3955 (3)	0.1091 (3)	0.0597 (11)
H28	−0.4565	0.4274	0.1066	0.072*
C29	−0.3156 (3)	0.4440 (3)	0.1037 (3)	0.0512 (10)
H29	−0.3167	0.5090	0.0973	0.061*
C30	−0.2305 (3)	0.3962 (2)	0.1079 (2)	0.0370 (8)
C31	−0.1365 (3)	0.4431 (2)	0.1060 (2)	0.0380 (8)
C32	−0.1273 (3)	0.5395 (3)	0.0946 (3)	0.0538 (10)
H32	−0.1810	0.5777	0.0872	0.065*
C33	−0.0376 (4)	0.5775 (3)	0.0945 (3)	0.0632 (12)
H33	−0.0301	0.6421	0.0886	0.076*
C34	0.0409 (3)	0.5200 (3)	0.1030 (3)	0.0568 (11)
H34	0.1020	0.5444	0.1018	0.068*
C35	0.0266 (3)	0.4249 (3)	0.1136 (2)	0.0506 (10)
H35	0.0796	0.3856	0.1199	0.061*
B1	0.3098 (4)	0.4133 (5)	0.0985 (3)	0.0656 (15)
B2	0.7926 (6)	0.9894 (5)	0.1737 (4)	0.0788 (17)
F1	0.2382 (3)	0.3522 (3)	0.0919 (4)	0.187 (3)
F2	0.2729 (3)	0.5017 (2)	0.1047 (2)	0.0951 (10)
F3	0.3600 (4)	0.4047 (4)	0.0379 (2)	0.171 (2)
F4	0.3677 (3)	0.3941 (3)	0.1634 (2)	0.1181 (14)
F5	0.7456 (5)	0.9235 (4)	0.1292 (4)	0.183 (2)
F6	0.7409 (3)	1.0311 (4)	0.2257 (2)	0.156 (2)

F7	0.8184 (3)	1.0528 (3)	0.1205 (2)	0.1159 (14)
F8	0.8733 (4)	0.9568 (4)	0.2117 (2)	0.174 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0358 (3)	0.0355 (3)	0.0441 (3)	0.00386 (18)	0.00372 (19)	0.00339 (18)
Fe1	0.0371 (3)	0.0374 (3)	0.0441 (3)	0.0001 (2)	0.0077 (2)	−0.0013 (2)
N1	0.0397 (17)	0.0382 (16)	0.0429 (16)	−0.0047 (14)	0.0007 (14)	0.0054 (13)
N2	0.0375 (16)	0.0342 (15)	0.0372 (15)	0.0025 (12)	0.0028 (12)	0.0016 (12)
N3	0.0423 (17)	0.0361 (16)	0.0423 (16)	0.0027 (14)	0.0078 (14)	0.0012 (12)
N4	0.0338 (16)	0.0355 (16)	0.0512 (18)	−0.0028 (13)	0.0042 (14)	0.0011 (13)
N5	0.0326 (16)	0.0387 (16)	0.0473 (17)	−0.0037 (13)	−0.0001 (13)	0.0009 (13)
C1	0.041 (2)	0.046 (2)	0.051 (2)	−0.0065 (17)	−0.0030 (18)	0.0115 (17)
C2	0.054 (3)	0.058 (3)	0.051 (2)	−0.016 (2)	−0.011 (2)	0.020 (2)
C3	0.073 (3)	0.053 (2)	0.040 (2)	−0.012 (2)	0.001 (2)	0.0071 (18)
C4	0.064 (3)	0.044 (2)	0.041 (2)	0.0012 (19)	0.0055 (19)	0.0037 (16)
C5	0.044 (2)	0.0311 (17)	0.0402 (18)	−0.0035 (15)	−0.0019 (16)	0.0017 (14)
C6	0.044 (2)	0.0347 (18)	0.0382 (18)	−0.0020 (15)	0.0049 (16)	0.0024 (14)
C7	0.044 (2)	0.0346 (18)	0.0393 (18)	0.0037 (15)	0.0106 (16)	0.0007 (14)
C8	0.038 (2)	0.0330 (17)	0.0440 (19)	−0.0044 (15)	0.0083 (16)	0.0048 (15)
C9	0.0369 (19)	0.0389 (19)	0.0403 (18)	0.0001 (15)	0.0033 (15)	0.0049 (15)
C10	0.040 (2)	0.0318 (17)	0.0378 (18)	−0.0022 (15)	0.0058 (15)	0.0011 (14)
C11	0.043 (2)	0.0316 (17)	0.0414 (19)	−0.0042 (15)	0.0088 (16)	−0.0003 (14)
C12	0.051 (2)	0.047 (2)	0.0389 (19)	−0.0004 (18)	0.0037 (17)	0.0033 (16)
C13	0.069 (3)	0.061 (3)	0.037 (2)	−0.006 (2)	0.009 (2)	−0.0006 (18)
C14	0.064 (3)	0.062 (3)	0.049 (2)	0.000 (2)	0.023 (2)	−0.009 (2)
C15	0.048 (2)	0.050 (2)	0.057 (2)	0.0066 (18)	0.013 (2)	−0.0089 (18)
C16	0.037 (2)	0.0329 (18)	0.048 (2)	0.0008 (15)	0.0086 (16)	0.0038 (15)
C17	0.044 (2)	0.0376 (19)	0.048 (2)	−0.0005 (16)	0.0051 (17)	−0.0039 (16)
C18	0.048 (2)	0.0355 (19)	0.062 (2)	0.0044 (17)	0.0149 (19)	−0.0024 (17)
C19	0.049 (2)	0.042 (2)	0.065 (3)	0.0098 (18)	0.010 (2)	0.0145 (19)
C20	0.042 (2)	0.044 (2)	0.049 (2)	0.0054 (17)	0.0108 (17)	0.0120 (17)
C21	0.053 (3)	0.041 (2)	0.124 (4)	−0.005 (2)	0.012 (3)	−0.003 (2)
C22	0.072 (3)	0.058 (3)	0.070 (3)	−0.022 (2)	0.005 (2)	0.009 (2)
C23	0.052 (3)	0.058 (3)	0.074 (3)	−0.015 (2)	0.022 (2)	−0.008 (2)
C24	0.051 (3)	0.071 (3)	0.068 (3)	−0.016 (2)	−0.003 (2)	−0.012 (2)
C25	0.069 (3)	0.060 (3)	0.082 (3)	−0.017 (2)	0.020 (3)	−0.033 (2)
C26	0.044 (2)	0.042 (2)	0.074 (3)	−0.0090 (18)	0.008 (2)	−0.0013 (19)
C27	0.036 (2)	0.064 (3)	0.082 (3)	−0.014 (2)	0.007 (2)	−0.003 (2)
C28	0.034 (2)	0.070 (3)	0.075 (3)	0.006 (2)	0.002 (2)	−0.006 (2)
C29	0.041 (2)	0.043 (2)	0.068 (3)	0.0054 (18)	0.001 (2)	0.0006 (19)
C30	0.0360 (19)	0.0361 (18)	0.0386 (18)	−0.0017 (15)	0.0025 (15)	0.0027 (14)
C31	0.0361 (19)	0.0343 (18)	0.0432 (18)	−0.0001 (15)	0.0020 (15)	0.0064 (15)
C32	0.047 (2)	0.036 (2)	0.078 (3)	0.0011 (18)	0.008 (2)	0.010 (2)
C33	0.061 (3)	0.042 (2)	0.086 (3)	−0.017 (2)	0.005 (3)	0.007 (2)
C34	0.045 (3)	0.058 (3)	0.067 (3)	−0.018 (2)	0.005 (2)	0.005 (2)
C35	0.034 (2)	0.060 (3)	0.058 (2)	−0.0026 (18)	0.0016 (18)	0.0054 (19)

B1	0.044 (3)	0.089 (4)	0.064 (3)	0.018 (3)	0.005 (2)	−0.015 (3)
B2	0.084 (4)	0.090 (4)	0.064 (3)	0.015 (3)	0.016 (3)	0.011 (3)
F1	0.062 (2)	0.101 (3)	0.390 (8)	−0.003 (2)	−0.013 (4)	−0.062 (4)
F2	0.077 (2)	0.081 (2)	0.126 (3)	0.0149 (17)	0.003 (2)	−0.0155 (19)
F3	0.188 (5)	0.254 (6)	0.080 (2)	0.114 (4)	0.061 (3)	0.028 (3)
F4	0.136 (4)	0.135 (3)	0.078 (2)	0.035 (3)	−0.021 (2)	−0.007 (2)
F5	0.226 (6)	0.130 (4)	0.192 (5)	−0.100 (4)	0.013 (4)	−0.006 (3)
F6	0.122 (4)	0.258 (6)	0.096 (3)	0.089 (4)	0.043 (3)	0.024 (3)
F7	0.150 (4)	0.114 (3)	0.082 (2)	−0.055 (3)	0.002 (2)	0.006 (2)
F8	0.177 (5)	0.263 (6)	0.085 (3)	0.149 (4)	0.026 (3)	0.029 (3)

Geometric parameters (Å, °)

Cu1—N2	1.928 (3)	C14—C15	1.374 (6)
Cu1—N4	1.983 (3)	C14—H14	0.9300
Cu1—N3	2.038 (3)	C15—H15	0.9300
Cu1—N1	2.062 (3)	C16—C20	1.432 (5)
Cu1—N5	2.195 (3)	C16—C17	1.436 (5)
Fe1—C25	2.020 (4)	C17—C18	1.410 (5)
Fe1—C21	2.023 (5)	C17—H17	0.9300
Fe1—C16	2.026 (4)	C18—C19	1.418 (6)
Fe1—C22	2.031 (5)	C18—H18	0.9300
Fe1—C24	2.035 (4)	C19—C20	1.427 (5)
Fe1—C17	2.036 (4)	C19—H19	0.9300
Fe1—C20	2.040 (4)	C20—H20	0.9300
Fe1—C23	2.047 (4)	C21—C22	1.403 (7)
Fe1—C19	2.049 (4)	C21—C25	1.406 (7)
Fe1—C18	2.051 (4)	C21—H21	0.9300
N1—C1	1.342 (5)	C22—C23	1.401 (7)
N1—C5	1.346 (5)	C22—H22	0.9300
N2—C10	1.344 (4)	C23—C24	1.396 (6)
N2—C6	1.345 (4)	C23—H23	0.9300
N3—C15	1.335 (5)	C24—C25	1.393 (7)
N3—C11	1.352 (5)	C24—H24	0.9300
N4—C26	1.342 (5)	C25—H25	0.9300
N4—C30	1.356 (4)	C26—C27	1.371 (6)
N5—C35	1.336 (5)	C26—H26	0.9300
N5—C31	1.339 (5)	C27—C28	1.350 (6)
C1—C2	1.373 (6)	C27—H27	0.9300
C1—H1	0.9300	C28—C29	1.367 (6)
C2—C3	1.366 (7)	C28—H28	0.9300
C2—H2	0.9300	C29—C30	1.373 (5)
C3—C4	1.389 (6)	C29—H29	0.9300
C3—H3	0.9300	C30—C31	1.484 (5)
C4—C5	1.376 (5)	C31—C32	1.392 (5)
C4—H4	0.9300	C32—C33	1.374 (6)
C5—C6	1.493 (5)	C32—H32	0.9300
C6—C7	1.376 (5)	C33—C34	1.370 (7)
C7—C8	1.403 (5)	C33—H33	0.9300

C7—H7	0.9300	C34—C35	1.380 (6)
C8—C9	1.397 (5)	C34—H34	0.9300
C8—C16	1.463 (5)	C35—H35	0.9300
C9—C10	1.377 (5)	B1—F3	1.306 (6)
C9—H9	0.9300	B1—F1	1.326 (7)
C10—C11	1.487 (5)	B1—F4	1.333 (7)
C11—C12	1.377 (5)	B1—F2	1.367 (7)
C12—C13	1.385 (6)	B2—F6	1.333 (8)
C12—H12	0.9300	B2—F8	1.334 (8)
C13—C14	1.362 (6)	B2—F5	1.336 (9)
C13—H13	0.9300	B2—F7	1.348 (7)
N2—Cu1—N4	170.84 (12)	C13—C14—C15	119.4 (4)
N2—Cu1—N3	80.08 (12)	C13—C14—H14	120.3
N4—Cu1—N3	99.41 (13)	C15—C14—H14	120.3
N2—Cu1—N1	79.52 (12)	N3—C15—C14	122.2 (4)
N4—Cu1—N1	99.40 (13)	N3—C15—H15	118.9
N3—Cu1—N1	157.97 (12)	C14—C15—H15	118.9
N2—Cu1—N5	110.34 (12)	C20—C16—C17	107.1 (3)
N4—Cu1—N5	78.78 (12)	C20—C16—C8	126.1 (3)
N3—Cu1—N5	100.77 (11)	C17—C16—C8	126.8 (3)
N1—Cu1—N5	94.03 (11)	C20—C16—Fe1	69.9 (2)
C25—Fe1—C21	40.7 (2)	C17—C16—Fe1	69.6 (2)
C25—Fe1—C16	120.98 (18)	C8—C16—Fe1	125.3 (2)
C21—Fe1—C16	107.16 (18)	C18—C17—C16	108.2 (3)
C25—Fe1—C22	68.0 (2)	C18—C17—Fe1	70.4 (2)
C21—Fe1—C22	40.5 (2)	C16—C17—Fe1	68.9 (2)
C16—Fe1—C22	124.61 (18)	C18—C17—H17	125.9
C25—Fe1—C24	40.2 (2)	C16—C17—H17	125.9
C21—Fe1—C24	67.9 (2)	Fe1—C17—H17	126.3
C16—Fe1—C24	156.34 (17)	C17—C18—C19	108.9 (3)
C22—Fe1—C24	67.7 (2)	C17—C18—Fe1	69.2 (2)
C25—Fe1—C17	156.7 (2)	C19—C18—Fe1	69.7 (2)
C21—Fe1—C17	120.89 (19)	C17—C18—H18	125.6
C16—Fe1—C17	41.42 (14)	C19—C18—H18	125.6
C22—Fe1—C17	107.37 (18)	Fe1—C18—H18	127.1
C24—Fe1—C17	161.26 (18)	C18—C19—C20	107.6 (4)
C25—Fe1—C20	108.12 (19)	C18—C19—Fe1	69.8 (2)
C21—Fe1—C20	125.35 (19)	C20—C19—Fe1	69.2 (2)
C16—Fe1—C20	41.23 (15)	C18—C19—H19	126.2
C22—Fe1—C20	162.26 (19)	C20—C19—H19	126.2
C24—Fe1—C20	121.37 (19)	Fe1—C19—H19	126.3
C17—Fe1—C20	68.93 (16)	C19—C20—C16	108.2 (3)
C25—Fe1—C23	67.49 (19)	C19—C20—Fe1	69.9 (2)
C21—Fe1—C23	67.7 (2)	C16—C20—Fe1	68.9 (2)
C16—Fe1—C23	161.66 (18)	C19—C20—H20	125.9
C22—Fe1—C23	40.2 (2)	C16—C20—H20	125.9
C24—Fe1—C23	39.99 (18)	Fe1—C20—H20	126.9
C17—Fe1—C23	124.69 (17)	C22—C21—C25	107.5 (5)
C20—Fe1—C23	156.05 (18)	C22—C21—Fe1	70.0 (3)

C25—Fe1—C19	125.3 (2)	C25—C21—Fe1	69.5 (3)
C21—Fe1—C19	162.4 (2)	C22—C21—H21	126.2
C16—Fe1—C19	69.28 (16)	C25—C21—H21	126.2
C22—Fe1—C19	155.5 (2)	Fe1—C21—H21	125.8
C24—Fe1—C19	108.0 (2)	C23—C22—C21	108.0 (5)
C17—Fe1—C19	68.55 (17)	C23—C22—Fe1	70.5 (3)
C20—Fe1—C19	40.85 (15)	C21—C22—Fe1	69.5 (3)
C23—Fe1—C19	120.97 (19)	C23—C22—H22	126.0
C25—Fe1—C18	161.9 (2)	C21—C22—H22	126.0
C21—Fe1—C18	155.8 (2)	Fe1—C22—H22	125.6
C16—Fe1—C18	68.86 (15)	C24—C23—C22	108.0 (4)
C22—Fe1—C18	120.87 (19)	C24—C23—Fe1	69.5 (3)
C24—Fe1—C18	125.24 (19)	C22—C23—Fe1	69.3 (3)
C17—Fe1—C18	40.37 (16)	C24—C23—H23	126.0
C20—Fe1—C18	68.30 (16)	C22—C23—H23	126.0
C23—Fe1—C18	108.13 (18)	Fe1—C23—H23	126.8
C19—Fe1—C18	40.46 (17)	C25—C24—C23	108.2 (5)
C1—N1—C5	118.1 (3)	C25—C24—Fe1	69.3 (3)
C1—N1—Cu1	127.9 (3)	C23—C24—Fe1	70.5 (3)
C5—N1—Cu1	114.0 (2)	C25—C24—H24	125.9
C10—N2—C6	120.6 (3)	C23—C24—H24	125.9
C10—N2—Cu1	119.3 (2)	Fe1—C24—H24	125.9
C6—N2—Cu1	119.9 (2)	C24—C25—C21	108.2 (5)
C15—N3—C11	118.6 (3)	C24—C25—Fe1	70.5 (2)
C15—N3—Cu1	127.3 (3)	C21—C25—Fe1	69.8 (3)
C11—N3—Cu1	114.0 (2)	C24—C25—H25	125.9
C26—N4—C30	118.2 (3)	C21—C25—H25	125.9
C26—N4—Cu1	123.7 (3)	Fe1—C25—H25	125.4
C30—N4—Cu1	118.1 (2)	N4—C26—C27	122.2 (4)
C35—N5—C31	118.7 (3)	N4—C26—H26	118.9
C35—N5—Cu1	129.7 (3)	C27—C26—H26	118.9
C31—N5—Cu1	111.3 (2)	C28—C27—C26	119.2 (4)
N1—C1—C2	122.5 (4)	C28—C27—H27	120.4
N1—C1—H1	118.8	C26—C27—H27	120.4
C2—C1—H1	118.8	C27—C28—C29	119.7 (4)
C3—C2—C1	119.4 (4)	C27—C28—H28	120.1
C3—C2—H2	120.3	C29—C28—H28	120.1
C1—C2—H2	120.3	C28—C29—C30	119.6 (4)
C2—C3—C4	118.9 (4)	C28—C29—H29	120.2
C2—C3—H3	120.6	C30—C29—H29	120.2
C4—C3—H3	120.6	N4—C30—C29	121.0 (3)
C5—C4—C3	118.9 (4)	N4—C30—C31	115.5 (3)
C5—C4—H4	120.6	C29—C30—C31	123.5 (3)
C3—C4—H4	120.6	N5—C31—C32	121.3 (4)
N1—C5—C4	122.2 (3)	N5—C31—C30	116.0 (3)
N1—C5—C6	114.3 (3)	C32—C31—C30	122.7 (3)
C4—C5—C6	123.5 (4)	C33—C32—C31	119.1 (4)
N2—C6—C7	121.2 (3)	C33—C32—H32	120.5
N2—C6—C5	112.2 (3)	C31—C32—H32	120.5

C7—C6—C5	126.6 (3)	C34—C33—C32	119.8 (4)
C6—C7—C8	119.4 (3)	C34—C33—H33	120.1
C6—C7—H7	120.3	C32—C33—H33	120.1
C8—C7—H7	120.3	C33—C34—C35	118.1 (4)
C9—C8—C7	118.0 (3)	C33—C34—H34	120.9
C9—C8—C16	121.0 (3)	C35—C34—H34	120.9
C7—C8—C16	121.0 (3)	N5—C35—C34	123.0 (4)
C10—C9—C8	120.0 (3)	N5—C35—H35	118.5
C10—C9—H9	120.0	C34—C35—H35	118.5
C8—C9—H9	120.0	F3—B1—F1	109.7 (6)
N2—C10—C9	120.7 (3)	F3—B1—F4	107.2 (5)
N2—C10—C11	112.2 (3)	F1—B1—F4	109.5 (6)
C9—C10—C11	127.0 (3)	F3—B1—F2	112.6 (6)
N3—C11—C12	121.6 (3)	F1—B1—F2	108.4 (4)
N3—C11—C10	114.3 (3)	F4—B1—F2	109.3 (5)
C12—C11—C10	124.0 (4)	F6—B2—F8	109.2 (5)
C11—C12—C13	118.8 (4)	F6—B2—F5	114.3 (7)
C11—C12—H12	120.6	F8—B2—F5	112.5 (7)
C13—C12—H12	120.6	F6—B2—F7	110.1 (6)
C14—C13—C12	119.3 (4)	F8—B2—F7	106.5 (6)
C14—C13—H13	120.4	F5—B2—F7	103.9 (5)
C12—C13—H13	120.4		
N2—Cu1—N1—C1	178.9 (3)	C22—Fe1—C19—C18	−48.1 (6)
N4—Cu1—N1—C1	8.1 (3)	C24—Fe1—C19—C18	−123.6 (3)
N3—Cu1—N1—C1	156.5 (3)	C17—Fe1—C19—C18	36.8 (2)
N5—Cu1—N1—C1	−71.2 (3)	C20—Fe1—C19—C18	119.0 (4)
N2—Cu1—N1—C5	−4.0 (2)	C23—Fe1—C19—C18	−81.7 (3)
N4—Cu1—N1—C5	−174.7 (2)	C25—Fe1—C19—C20	76.3 (3)
N3—Cu1—N1—C5	−26.3 (5)	C21—Fe1—C19—C20	43.7 (7)
N5—Cu1—N1—C5	106.0 (2)	C16—Fe1—C19—C20	−37.6 (2)
N3—Cu1—N2—C10	−0.8 (3)	C22—Fe1—C19—C20	−167.1 (4)
N1—Cu1—N2—C10	−172.5 (3)	C24—Fe1—C19—C20	117.4 (3)
N5—Cu1—N2—C10	97.1 (3)	C17—Fe1—C19—C20	−82.2 (3)
N3—Cu1—N2—C6	174.5 (3)	C23—Fe1—C19—C20	159.3 (2)
N1—Cu1—N2—C6	2.8 (3)	C18—Fe1—C19—C20	−119.0 (4)
N5—Cu1—N2—C6	−87.6 (3)	C18—C19—C20—C16	−1.2 (4)
N2—Cu1—N3—C15	−178.5 (3)	Fe1—C19—C20—C16	58.3 (3)
N4—Cu1—N3—C15	−7.7 (3)	C18—C19—C20—Fe1	−59.5 (3)
N1—Cu1—N3—C15	−156.1 (3)	C17—C16—C20—C19	1.0 (4)
N5—Cu1—N3—C15	72.5 (3)	C8—C16—C20—C19	−178.6 (3)
N2—Cu1—N3—C11	0.9 (2)	Fe1—C16—C20—C19	−59.0 (3)
N4—Cu1—N3—C11	171.6 (2)	C17—C16—C20—Fe1	60.0 (2)
N1—Cu1—N3—C11	23.2 (5)	C8—C16—C20—Fe1	−119.6 (4)
N5—Cu1—N3—C11	−108.1 (2)	C25—Fe1—C20—C19	−123.4 (3)
N3—Cu1—N4—C26	−77.3 (3)	C21—Fe1—C20—C19	−165.2 (3)
N1—Cu1—N4—C26	91.2 (3)	C16—Fe1—C20—C19	119.9 (3)
N5—Cu1—N4—C26	−176.6 (3)	C22—Fe1—C20—C19	162.3 (6)
N3—Cu1—N4—C30	103.6 (3)	C24—Fe1—C20—C19	−81.3 (3)
N1—Cu1—N4—C30	−87.9 (3)	C17—Fe1—C20—C19	81.2 (3)

N5—Cu1—N4—C30	4.4 (3)	C23—Fe1—C20—C19	−48.3 (5)
N2—Cu1—N5—C35	0.2 (4)	C18—Fe1—C20—C19	37.7 (3)
N4—Cu1—N5—C35	−178.9 (4)	C25—Fe1—C20—C16	116.6 (3)
N3—Cu1—N5—C35	83.5 (3)	C21—Fe1—C20—C16	74.9 (3)
N1—Cu1—N5—C35	−80.1 (3)	C22—Fe1—C20—C16	42.4 (7)
N2—Cu1—N5—C31	174.1 (2)	C24—Fe1—C20—C16	158.7 (2)
N4—Cu1—N5—C31	−5.0 (2)	C17—Fe1—C20—C16	−38.8 (2)
N3—Cu1—N5—C31	−102.6 (3)	C23—Fe1—C20—C16	−168.2 (4)
N1—Cu1—N5—C31	93.8 (3)	C19—Fe1—C20—C16	−119.9 (3)
C5—N1—C1—C2	1.0 (5)	C18—Fe1—C20—C16	−82.3 (2)
Cu1—N1—C1—C2	178.0 (3)	C25—Fe1—C21—C22	118.5 (4)
N1—C1—C2—C3	−0.9 (6)	C16—Fe1—C21—C22	−123.6 (3)
C1—C2—C3—C4	−0.2 (6)	C24—Fe1—C21—C22	81.0 (3)
C2—C3—C4—C5	1.3 (6)	C17—Fe1—C21—C22	−80.5 (3)
C1—N1—C5—C4	0.2 (5)	C20—Fe1—C21—C22	−165.4 (3)
Cu1—N1—C5—C4	−177.2 (3)	C23—Fe1—C21—C22	37.6 (3)
C1—N1—C5—C6	−178.2 (3)	C19—Fe1—C21—C22	160.9 (6)
Cu1—N1—C5—C6	4.4 (4)	C18—Fe1—C21—C22	−47.1 (6)
C3—C4—C5—N1	−1.4 (6)	C16—Fe1—C21—C25	117.8 (3)
C3—C4—C5—C6	176.9 (4)	C22—Fe1—C21—C25	−118.5 (4)
C10—N2—C6—C7	−3.6 (5)	C24—Fe1—C21—C25	−37.5 (3)
Cu1—N2—C6—C7	−178.9 (3)	C17—Fe1—C21—C25	161.0 (3)
C10—N2—C6—C5	173.9 (3)	C20—Fe1—C21—C25	76.1 (3)
Cu1—N2—C6—C5	−1.3 (4)	C23—Fe1—C21—C25	−80.9 (3)
N1—C5—C6—N2	−2.2 (4)	C19—Fe1—C21—C25	42.4 (8)
C4—C5—C6—N2	179.5 (3)	C18—Fe1—C21—C25	−165.7 (4)
N1—C5—C6—C7	175.2 (3)	C25—C21—C22—C23	−0.6 (5)
C4—C5—C6—C7	−3.1 (6)	Fe1—C21—C22—C23	−60.3 (3)
N2—C6—C7—C8	1.4 (5)	C25—C21—C22—Fe1	59.7 (3)
C5—C6—C7—C8	−175.8 (3)	C25—Fe1—C22—C23	80.7 (3)
C6—C7—C8—C9	1.0 (5)	C21—Fe1—C22—C23	118.9 (4)
C6—C7—C8—C16	178.4 (3)	C16—Fe1—C22—C23	−166.0 (3)
C7—C8—C9—C10	−1.1 (5)	C24—Fe1—C22—C23	37.1 (3)
C16—C8—C9—C10	−178.5 (3)	C17—Fe1—C22—C23	−123.6 (3)
C6—N2—C10—C9	3.5 (5)	C20—Fe1—C22—C23	161.4 (5)
Cu1—N2—C10—C9	178.8 (3)	C19—Fe1—C22—C23	−47.4 (6)
C6—N2—C10—C11	−174.7 (3)	C18—Fe1—C22—C23	−81.6 (3)
Cu1—N2—C10—C11	0.6 (4)	C25—Fe1—C22—C21	−38.2 (3)
C8—C9—C10—N2	−1.1 (5)	C16—Fe1—C22—C21	75.2 (3)
C8—C9—C10—C11	176.8 (3)	C24—Fe1—C22—C21	−81.7 (3)
C15—N3—C11—C12	−0.6 (5)	C17—Fe1—C22—C21	117.5 (3)
Cu1—N3—C11—C12	180.0 (3)	C20—Fe1—C22—C21	42.5 (7)
C15—N3—C11—C10	178.6 (3)	C23—Fe1—C22—C21	−118.9 (4)
Cu1—N3—C11—C10	−0.8 (4)	C19—Fe1—C22—C21	−166.2 (4)
N2—C10—C11—N3	0.2 (4)	C18—Fe1—C22—C21	159.5 (3)
C9—C10—C11—N3	−177.8 (3)	C21—C22—C23—C24	0.7 (5)
N2—C10—C11—C12	179.4 (3)	Fe1—C22—C23—C24	−58.9 (3)
C9—C10—C11—C12	1.3 (6)	C21—C22—C23—Fe1	59.6 (3)
N3—C11—C12—C13	1.3 (6)	C25—Fe1—C23—C24	37.6 (3)

C10—C11—C12—C13	−177.8 (3)	C21—Fe1—C23—C24	81.7 (3)
C11—C12—C13—C14	−1.0 (6)	C16—Fe1—C23—C24	158.9 (5)
C12—C13—C14—C15	0.0 (7)	C22—Fe1—C23—C24	119.6 (4)
C11—N3—C15—C14	−0.4 (6)	C17—Fe1—C23—C24	−165.2 (3)
Cu1—N3—C15—C14	178.9 (3)	C20—Fe1—C23—C24	−46.5 (5)
C13—C14—C15—N3	0.8 (7)	C19—Fe1—C23—C24	−81.2 (3)
C9—C8—C16—C20	−4.6 (6)	C18—Fe1—C23—C24	−123.7 (3)
C7—C8—C16—C20	178.1 (3)	C25—Fe1—C23—C22	−82.1 (3)
C9—C8—C16—C17	175.8 (3)	C21—Fe1—C23—C22	−37.9 (3)
C7—C8—C16—C17	−1.5 (6)	C16—Fe1—C23—C22	39.3 (7)
C9—C8—C16—Fe1	−94.4 (4)	C24—Fe1—C23—C22	−119.6 (4)
C7—C8—C16—Fe1	88.3 (4)	C17—Fe1—C23—C22	75.1 (3)
C25—Fe1—C16—C20	−82.3 (3)	C20—Fe1—C23—C22	−166.1 (4)
C21—Fe1—C16—C20	−124.5 (3)	C19—Fe1—C23—C22	159.2 (3)
C22—Fe1—C16—C20	−165.6 (3)	C18—Fe1—C23—C22	116.7 (3)
C24—Fe1—C16—C20	−50.5 (5)	C22—C23—C24—C25	−0.5 (5)
C17—Fe1—C16—C20	118.0 (3)	Fe1—C23—C24—C25	−59.3 (3)
C23—Fe1—C16—C20	164.7 (5)	C22—C23—C24—Fe1	58.8 (3)
C19—Fe1—C16—C20	37.3 (2)	C21—Fe1—C24—C25	38.0 (3)
C18—Fe1—C16—C20	80.8 (2)	C16—Fe1—C24—C25	−44.4 (6)
C25—Fe1—C16—C17	159.8 (3)	C22—Fe1—C24—C25	81.9 (4)
C21—Fe1—C16—C17	117.5 (3)	C17—Fe1—C24—C25	159.9 (5)
C22—Fe1—C16—C17	76.5 (3)	C20—Fe1—C24—C25	−80.9 (4)
C24—Fe1—C16—C17	−168.5 (4)	C23—Fe1—C24—C25	119.2 (5)
C20—Fe1—C16—C17	−118.0 (3)	C19—Fe1—C24—C25	−123.8 (3)
C23—Fe1—C16—C17	46.7 (6)	C18—Fe1—C24—C25	−165.2 (3)
C19—Fe1—C16—C17	−80.7 (2)	C25—Fe1—C24—C23	−119.2 (5)
C18—Fe1—C16—C17	−37.2 (2)	C21—Fe1—C24—C23	−81.2 (3)
C25—Fe1—C16—C8	38.4 (4)	C16—Fe1—C24—C23	−163.6 (4)
C21—Fe1—C16—C8	−3.8 (4)	C22—Fe1—C24—C23	−37.3 (3)
C22—Fe1—C16—C8	−44.9 (4)	C17—Fe1—C24—C23	40.7 (7)
C24—Fe1—C16—C8	70.2 (6)	C20—Fe1—C24—C23	159.8 (3)
C17—Fe1—C16—C8	−121.3 (4)	C19—Fe1—C24—C23	117.0 (3)
C20—Fe1—C16—C8	120.7 (4)	C18—Fe1—C24—C23	75.6 (3)
C23—Fe1—C16—C8	−74.6 (6)	C23—C24—C25—C21	0.2 (5)
C19—Fe1—C16—C8	158.0 (4)	Fe1—C24—C25—C21	−59.8 (3)
C18—Fe1—C16—C8	−158.5 (4)	C23—C24—C25—Fe1	60.0 (3)
C20—C16—C17—C18	−0.5 (4)	C22—C21—C25—C24	0.3 (5)
C8—C16—C17—C18	179.2 (3)	Fe1—C21—C25—C24	60.3 (3)
Fe1—C16—C17—C18	59.7 (3)	C22—C21—C25—Fe1	−60.0 (3)
C20—C16—C17—Fe1	−60.2 (3)	C21—Fe1—C25—C24	−118.9 (5)
C8—C16—C17—Fe1	119.5 (4)	C16—Fe1—C25—C24	160.9 (3)
C25—Fe1—C17—C18	−167.9 (5)	C22—Fe1—C25—C24	−81.0 (3)
C21—Fe1—C17—C18	159.7 (3)	C17—Fe1—C25—C24	−163.8 (4)
C16—Fe1—C17—C18	−119.5 (3)	C20—Fe1—C25—C24	117.5 (3)
C22—Fe1—C17—C18	117.5 (3)	C23—Fe1—C25—C24	−37.4 (3)
C24—Fe1—C17—C18	46.1 (6)	C19—Fe1—C25—C24	75.5 (4)
C20—Fe1—C17—C18	−80.9 (2)	C18—Fe1—C25—C24	42.0 (7)
C23—Fe1—C17—C18	76.7 (3)	C16—Fe1—C25—C21	−80.2 (3)

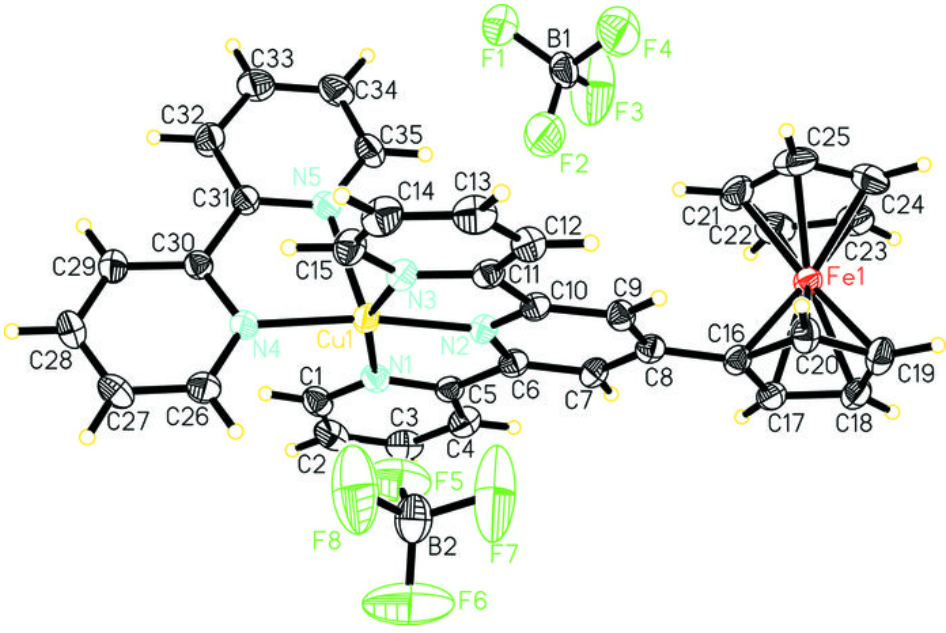
C19—Fe1—C17—C18	−36.9 (2)	C22—Fe1—C25—C21	38.0 (3)
C25—Fe1—C17—C16	−48.4 (6)	C24—Fe1—C25—C21	118.9 (5)
C21—Fe1—C17—C16	−80.9 (3)	C17—Fe1—C25—C21	−44.9 (6)
C22—Fe1—C17—C16	−123.0 (2)	C20—Fe1—C25—C21	−123.6 (3)
C24—Fe1—C17—C16	165.5 (5)	C23—Fe1—C25—C21	81.5 (3)
C20—Fe1—C17—C16	38.6 (2)	C19—Fe1—C25—C21	−165.6 (3)
C23—Fe1—C17—C16	−163.8 (2)	C18—Fe1—C25—C21	161.0 (5)
C19—Fe1—C17—C16	82.6 (2)	C30—N4—C26—C27	−0.3 (6)
C18—Fe1—C17—C16	119.5 (3)	Cu1—N4—C26—C27	−179.3 (3)
C16—C17—C18—C19	−0.3 (4)	N4—C26—C27—C28	0.4 (7)
Fe1—C17—C18—C19	58.5 (3)	C26—C27—C28—C29	−0.1 (7)
C16—C17—C18—Fe1	−58.8 (2)	C27—C28—C29—C30	−0.3 (7)
C25—Fe1—C18—C17	164.5 (6)	C26—N4—C30—C29	−0.2 (5)
C21—Fe1—C18—C17	−46.8 (5)	Cu1—N4—C30—C29	178.9 (3)
C16—Fe1—C18—C17	38.1 (2)	C26—N4—C30—C31	177.8 (3)
C22—Fe1—C18—C17	−80.4 (3)	Cu1—N4—C30—C31	−3.1 (4)
C24—Fe1—C18—C17	−163.5 (3)	C28—C29—C30—N4	0.5 (6)
C20—Fe1—C18—C17	82.6 (2)	C28—C29—C30—C31	−177.3 (4)
C23—Fe1—C18—C17	−122.6 (3)	C35—N5—C31—C32	0.2 (6)
C19—Fe1—C18—C17	120.6 (3)	Cu1—N5—C31—C32	−174.4 (3)
C25—Fe1—C18—C19	43.9 (7)	C35—N5—C31—C30	179.6 (3)
C21—Fe1—C18—C19	−167.4 (4)	Cu1—N5—C31—C30	4.9 (4)
C16—Fe1—C18—C19	−82.5 (3)	N4—C30—C31—N5	−1.6 (5)
C22—Fe1—C18—C19	159.0 (3)	C29—C30—C31—N5	176.3 (4)
C24—Fe1—C18—C19	75.9 (3)	N4—C30—C31—C32	177.7 (4)
C17—Fe1—C18—C19	−120.6 (3)	C29—C30—C31—C32	−4.4 (6)
C20—Fe1—C18—C19	−38.0 (2)	N5—C31—C32—C33	−1.3 (6)
C23—Fe1—C18—C19	116.8 (3)	C30—C31—C32—C33	179.4 (4)
C17—C18—C19—C20	0.9 (4)	C31—C32—C33—C34	2.0 (7)
Fe1—C18—C19—C20	59.1 (3)	C32—C33—C34—C35	−1.6 (7)
C17—C18—C19—Fe1	−58.3 (3)	C31—N5—C35—C34	0.2 (6)
C25—Fe1—C19—C18	−164.7 (3)	Cu1—N5—C35—C34	173.7 (3)
C21—Fe1—C19—C18	162.7 (6)	C33—C34—C35—N5	0.5 (7)
C16—Fe1—C19—C18	81.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F4^{i}	0.93	2.51	3.306 (5)	143
C4—H4···F8^{ii}	0.93	2.40	3.176 (6)	141
C17—H17···F7^{ii}	0.93	2.39	3.296 (5)	165
C13—H13···F3^{iii}	0.93	2.54	3.140 (6)	123
C34—H34···F2	0.93	2.48	3.274 (6)	144
C35—H35···F1	0.93	2.37	3.208 (6)	149

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

Fig. 1


F1
B1
F4
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N5
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C15
C11
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C26
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C2
F5
F8
B2
F7
F6
C25
C21
C24
C22
C23
Fe1
C16
C20
C19
C17
C18