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Aquabis(2,2′-bipyridine-κ^2N,N')-copper(II) bis(tetrafluoridoborate)

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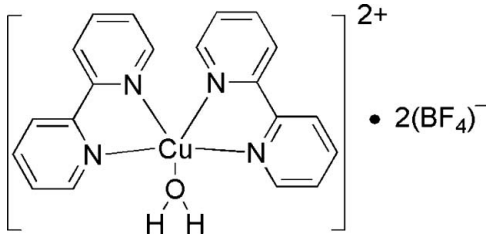
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in solvent or counterion; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 11.3.

In the title compound, $[Cu(C_{10}H_8N_2)_2(H_2O)](BF_4)_2$, the Cu^{II} atom is coordinated by four N atoms and one O atom in a distorted trigonal–bipyramidal geometry. The Cu—N bond lengths are in the range 1.982 (3)–2.124 (3) Å, while the Cu—O distance is 2.035 (4) Å. The structure is stabilized by O—H···F hydrogen bonds between the Cu^{II} complex and the tetrafluoridoborate anion. The F atoms of one anion are disordered over two positions; the site occupancy ratio is *ca* 3:2.

Related literature

For related literature, see: Şerb *et al.* (2007); Sigman *et al.* (1979); Tomislav (2006); Xu *et al.* (2005).



Experimental

Crystal data

$[Cu(C_{10}H_8N_2)_2(H_2O)](BF_4)_2$
M_r = 567.54
Monoclinic, $P2_1/c$
a = 9.0961 (16) Å
b = 13.571 (2) Å
c = 19.338 (3) Å
β = 103.507 (3)°
V = 2321.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.780, T_{max} = 0.853
11615 measured reflections
4090 independent reflections
2549 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.02
4090 reflections
363 parameters
99 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.982 (3)	Cu1—N4	2.095 (4)
Cu1—N1	1.993 (3)	Cu1—N2	2.124 (3)
Cu1—O1	2.035 (4)		
N3—Cu1—N4	79.72 (14)	N1—Cu1—N2	79.47 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···F8^{i}	0.86	2.26	3.113 (4)	171
O1—H1B···F7^{ii}	0.86	2.44	3.038 (4)	127

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2015).

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supplementary materials

Acta Cryst. (2007). E**63**, m2380 [**doi:10.1107/S1600536807033557**]

Aquabis(2,2'-bipyridine-κ^2N,N')copper(II) bis(tetrafluoridoborate)

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Comment

Copper(II) coordination compounds have been investigated frequently, not only because of their interesting magnetic superexchange interactions, but also because of their relevance for bioinorganic model systems in copper enzymes (Sigman *et al.*, 1979). Here, the synthesis and crystal structure of the title bis(tetrafluoridoborate) complex, are reported.

The crystal structure of (I) consists of copper(II) complex cations and bis(tetrafluoridoborate) anions, as shown in Fig. 1. The Cu^{II} atom assumes a CuN_4O trigonal-bipyramidal coordination geometry formed by two N,*N*'-bidentate bpy ligands and one equatorial oxygen atom (Fig. 1). The Cu—N bond lengths are in the range 1.982 (3)–2.124 (3) Å, while the Cu—O bond distance is 2.035 (4) Å (Table 1). The Cu—N bond lengths in (I) are in agreement with those in previously characterized Cu—N bonds in $[Cu(bpy)_2]^{I}$ or $[Cu(phen)_2]^{II}$(Tomislav, 2006; Xu *et al.*, 2005; Şerb *et al.*, 2007). The bite angles in (I) are smaller than 90 °, which is due to the rigid geometry of the bidentate bpy ligand.

The interligand dihedral angle of 67.3 (3) ° in (I) is much lower than that found in $[Cu(bpy)_2]^{I}$ cited above (87.5 (11) °). The structure is stabilized by O—H···F type hydrogen bonds between the Cu^{II} complex and tetrafluoridoborate anion.

Experimental

A aqueous solution (15 ml) of $Cu(BF_4)_2$ (23.7 mg, 0.1 mmol) was added to the methanol solution (20 ml) of 1,10-phenanthroline (39.6 mg, 0.2 mmol) and stirred for a further 1 h. The solution was kept at room temperature and blue crystals were formed after a week (yield 35%).

Refinement

The H atoms were placed in caculated positions with C—H = 0.93 Å and O—H = 0.85 Å and were included in the refinement with U_{iso}(H) = 1.2U_{eq}(C/O). One of the BF_4 anions was found to be disordered oversites F1 - F4 and F1' - F4'. The site occupancies of F-atoms were determined using an isotropic model and the B—F distances were fixed at 1.36 (1) Å for both the anions in the subsequent refinement cycles.

Figures

Fig. 1. A view of complex (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Aquabis(2,2'-bipyridine-κ^2*N*,*N*')copper(II) bis(tetrafluoridoborate)

Crystal data

$[Cu(C_{10}H_8N_2)_2(H_2O)](BF_4)_2$	F_{000} = 1140
M_r = 567.54	D_x = 1.624 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2544 reflections
a = 9.0961 (16) Å	θ = 2.3–23.3º
b = 13.571 (2) Å	μ = 1.03 mm^{-1}
c = 19.338 (3) Å	T = 294 (2) K
β = 103.507 (3)º	Block, blue
V = 2321.1 (6) Å^3	0.24 × 0.20 × 0.16 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4090 independent reflections
Radiation source: fine-focus sealed tube	2549 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −10→10
T_{min} = 0.780, T_{max} = 0.853	k = −16→12
11615 measured reflections	l = −18→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.136	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 1.4025P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.003
4090 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
363 parameters	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
99 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0078 (8)

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}	Occ. (<1)
Cu1	0.94520 (6)	0.73629 (4)	0.86050 (3)	0.0429 (2)	
O1	0.9400 (4)	0.5864 (3)	0.86045 (18)	0.0758 (11)	
H1A	0.8685	0.5616	0.8775	0.091*	
H1B	1.0214	0.5516	0.8665	0.091*	
N1	1.0849 (4)	0.7371 (2)	0.79494 (19)	0.0451 (9)	
N2	0.8180 (4)	0.8221 (2)	0.77547 (17)	0.0419 (9)	
N3	0.8064 (4)	0.7459 (2)	0.92541 (18)	0.0398 (8)	
N4	1.0677 (4)	0.8328 (2)	0.93734 (18)	0.0432 (9)	
C1	1.2179 (5)	0.6899 (4)	0.8075 (3)	0.0615 (14)	
H1	1.2488	0.6553	0.8499	0.074*	
C2	1.3106 (6)	0.6902 (4)	0.7609 (3)	0.0652 (14)	
H2	1.4019	0.6563	0.7714	0.078*	
C3	1.2659 (6)	0.7414 (4)	0.6989 (3)	0.0596 (13)	
H3	1.3271	0.7438	0.6666	0.072*	
C4	1.1294 (6)	0.7893 (3)	0.6849 (2)	0.0532 (12)	
H4	1.0975	0.8242	0.6427	0.064*	
C5	1.0392 (5)	0.7859 (3)	0.7329 (2)	0.0384 (10)	
C6	0.8878 (5)	0.8317 (3)	0.7217 (2)	0.0389 (10)	
C7	0.8180 (6)	0.8806 (3)	0.6600 (2)	0.0500 (12)	
H7	0.8680	0.8880	0.6235	0.060*	
C8	0.6743 (6)	0.9182 (3)	0.6525 (3)	0.0589 (13)	
H8	0.6255	0.9498	0.6108	0.071*	
C9	0.6046 (6)	0.9080 (3)	0.7084 (3)	0.0587 (13)	
H9	0.5079	0.9329	0.7050	0.070*	
C10	0.6803 (5)	0.8605 (3)	0.7689 (2)	0.0500 (12)	
H10	0.6339	0.8549	0.8067	0.060*	
C11	0.6722 (5)	0.7006 (3)	0.9144 (2)	0.0514 (12)	
H11	0.6407	0.6623	0.8738	0.062*	
C12	0.5795 (5)	0.7083 (4)	0.9609 (3)	0.0583 (13)	
H12	0.4875	0.6753	0.9520	0.070*	
C13	0.6240 (6)	0.7651 (3)	1.0202 (3)	0.0568 (13)	
H13	0.5616	0.7725	1.0517	0.068*	
C14	0.7635 (5)	0.8118 (3)	1.0329 (2)	0.0510 (12)	

H14	0.7967	0.8499	1.0735	0.061*	
C15	0.8525 (5)	0.8009 (3)	0.9845 (2)	0.0384 (10)	
C16	1.0044 (5)	0.8465 (3)	0.9928 (2)	0.0401 (10)	
C17	1.0767 (6)	0.8993 (3)	1.0525 (2)	0.0536 (12)	
H17	1.0308	0.9078	1.0903	0.064*	
C18	1.2169 (6)	0.9387 (4)	1.0551 (3)	0.0678 (15)	
H18	1.2679	0.9736	1.0949	0.081*	
C19	1.2808 (6)	0.9257 (4)	0.9976 (3)	0.0685 (15)	
H19	1.3755	0.9520	0.9983	0.082*	
C20	1.2037 (5)	0.8736 (3)	0.9395 (3)	0.0550 (12)	
H20	1.2465	0.8665	0.9005	0.066*	
B1	0.6694 (6)	0.5485 (4)	0.6935 (3)	0.0659 (17)	
F1	0.8178 (9)	0.5433 (9)	0.6902 (8)	0.104 (4)	0.595 (11)
F2	0.5891 (10)	0.4695 (7)	0.6616 (5)	0.122 (4)	0.595 (11)
F3	0.5912 (11)	0.6298 (8)	0.6588 (6)	0.148 (4)	0.595 (11)
F4	0.6459 (12)	0.5574 (8)	0.7600 (4)	0.084 (3)	0.595 (11)
F1'	0.8079 (12)	0.5843 (11)	0.6883 (9)	0.077 (4)	0.405 (11)
F2'	0.6878 (18)	0.4499 (7)	0.7132 (8)	0.131 (5)	0.405 (11)
F3'	0.5836 (10)	0.5514 (11)	0.6293 (4)	0.095 (4)	0.405 (11)
F4'	0.633 (2)	0.5993 (11)	0.7463 (8)	0.101 (5)	0.405 (11)
B2	0.2352 (6)	0.5935 (4)	0.0273 (2)	0.0459 (13)	
F5	0.0851 (3)	0.6057 (2)	0.02780 (15)	0.0775 (9)	
F6	0.3119 (4)	0.6801 (2)	0.04648 (19)	0.0944 (11)	
F7	0.2497 (4)	0.5678 (3)	−0.03890 (15)	0.0938 (11)	
F8	0.2977 (4)	0.5252 (3)	0.07647 (19)	0.1033 (12)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0414 (3)	0.0536 (4)	0.0386 (3)	−0.0004 (3)	0.0190 (2)	0.0054 (3)
O1	0.070 (2)	0.072 (2)	0.090 (3)	−0.0009 (19)	0.028 (2)	0.006 (2)
N1	0.042 (2)	0.053 (2)	0.044 (2)	0.0051 (18)	0.0161 (17)	0.0097 (18)
N2	0.044 (2)	0.047 (2)	0.035 (2)	−0.0001 (17)	0.0100 (17)	0.0040 (16)
N3	0.040 (2)	0.048 (2)	0.0344 (19)	−0.0024 (16)	0.0143 (15)	0.0015 (16)
N4	0.039 (2)	0.043 (2)	0.048 (2)	−0.0009 (16)	0.0099 (18)	0.0100 (17)
C1	0.050 (3)	0.082 (4)	0.056 (3)	0.012 (3)	0.020 (3)	0.018 (3)
C2	0.047 (3)	0.086 (4)	0.070 (4)	0.008 (3)	0.028 (3)	0.002 (3)
C3	0.053 (3)	0.078 (4)	0.056 (3)	−0.012 (3)	0.030 (2)	−0.011 (3)
C4	0.062 (3)	0.065 (3)	0.039 (3)	−0.015 (3)	0.024 (2)	0.002 (2)
C5	0.045 (3)	0.040 (2)	0.032 (2)	−0.0089 (19)	0.0120 (19)	−0.0009 (18)
C6	0.047 (3)	0.036 (2)	0.035 (2)	−0.0085 (19)	0.012 (2)	0.0006 (19)
C7	0.062 (3)	0.051 (3)	0.039 (3)	−0.008 (2)	0.016 (2)	0.005 (2)
C8	0.066 (4)	0.056 (3)	0.048 (3)	0.000 (3)	−0.001 (3)	0.016 (2)
C9	0.055 (3)	0.050 (3)	0.066 (3)	0.009 (2)	0.004 (3)	0.006 (3)
C10	0.047 (3)	0.057 (3)	0.047 (3)	0.007 (2)	0.012 (2)	0.003 (2)
C11	0.046 (3)	0.064 (3)	0.048 (3)	−0.011 (2)	0.020 (2)	−0.005 (2)
C12	0.044 (3)	0.072 (3)	0.063 (3)	−0.010 (2)	0.022 (2)	0.005 (3)
C13	0.058 (3)	0.066 (3)	0.057 (3)	0.007 (3)	0.035 (3)	0.007 (3)

C14	0.063 (3)	0.054 (3)	0.040 (3)	0.003 (2)	0.020 (2)	0.003 (2)
C15	0.048 (3)	0.036 (2)	0.033 (2)	0.0040 (19)	0.014 (2)	0.0077 (19)
C16	0.047 (3)	0.030 (2)	0.041 (3)	0.0017 (19)	0.005 (2)	0.0058 (19)
C17	0.065 (3)	0.043 (3)	0.048 (3)	0.005 (2)	0.002 (2)	0.002 (2)
C18	0.068 (4)	0.049 (3)	0.075 (4)	−0.008 (3)	−0.005 (3)	−0.007 (3)
C19	0.049 (3)	0.052 (3)	0.097 (5)	−0.011 (2)	0.001 (3)	0.007 (3)
C20	0.043 (3)	0.055 (3)	0.067 (3)	−0.008 (2)	0.013 (3)	0.008 (3)
B1	0.069 (5)	0.082 (5)	0.052 (4)	0.006 (4)	0.024 (4)	0.015 (4)
F1	0.073 (5)	0.133 (8)	0.113 (6)	0.009 (4)	0.031 (4)	−0.023 (6)
F2	0.109 (6)	0.148 (7)	0.121 (7)	−0.030 (5)	0.048 (5)	−0.068 (5)
F3	0.161 (7)	0.160 (8)	0.134 (7)	0.027 (6)	0.057 (5)	0.061 (6)
F4	0.080 (5)	0.124 (7)	0.052 (4)	−0.020 (5)	0.023 (3)	−0.001 (4)
F1'	0.073 (7)	0.109 (9)	0.061 (6)	−0.009 (5)	0.036 (5)	0.009 (6)
F2'	0.159 (9)	0.102 (7)	0.150 (9)	0.033 (6)	0.072 (7)	0.056 (6)
F3'	0.070 (6)	0.139 (9)	0.061 (6)	−0.016 (6)	−0.018 (4)	0.010 (5)
F4'	0.085 (7)	0.103 (8)	0.122 (9)	0.016 (6)	0.039 (7)	−0.043 (7)
B2	0.051 (3)	0.053 (3)	0.037 (3)	−0.007 (3)	0.017 (3)	−0.001 (3)
F5	0.0545 (19)	0.113 (2)	0.068 (2)	−0.0087 (16)	0.0209 (15)	−0.0189 (17)
F6	0.095 (2)	0.080 (2)	0.120 (3)	−0.0336 (19)	0.049 (2)	−0.020 (2)
F7	0.082 (2)	0.152 (3)	0.0515 (19)	0.003 (2)	0.0243 (17)	−0.0254 (19)
F8	0.103 (3)	0.102 (3)	0.099 (3)	0.004 (2)	0.014 (2)	0.049 (2)

Geometric parameters (Å, °)

Cu1—N3	1.982 (3)	C10—H10	0.9300
Cu1—N1	1.993 (3)	C11—C12	1.372 (6)
Cu1—O1	2.035 (4)	C11—H11	0.9300
Cu1—N4	2.095 (4)	C12—C13	1.362 (7)
Cu1—N2	2.124 (3)	C12—H12	0.9300
O1—H1A	0.8635	C13—C14	1.389 (6)
O1—H1B	0.8629	C13—H13	0.9300
N1—C1	1.340 (6)	C14—C15	1.381 (6)
N1—C5	1.347 (5)	C14—H14	0.9300
N2—C10	1.335 (5)	C15—C16	1.488 (6)
N2—C6	1.345 (5)	C16—C17	1.387 (6)
N3—C11	1.339 (5)	C17—C18	1.373 (7)
N3—C15	1.347 (5)	C17—H17	0.9300
N4—C16	1.344 (5)	C18—C19	1.380 (7)
N4—C20	1.347 (5)	C18—H18	0.9300
C1—C2	1.371 (6)	C19—C20	1.374 (7)
C1—H1	0.9300	C19—H19	0.9300
C2—C3	1.362 (7)	C20—H20	0.9300
C2—H2	0.9300	B1—F3'	1.304 (7)
C3—C4	1.372 (7)	B1—F4'	1.339 (9)
C3—H3	0.9300	B1—F4	1.359 (8)
C4—C5	1.376 (6)	B1—F2	1.361 (7)
C4—H4	0.9300	B1—F1	1.368 (8)
C5—C6	1.480 (6)	B1—F1'	1.375 (9)
C6—C7	1.383 (6)	B1—F2'	1.391 (8)

C7—C8	1.379 (6)	B1—F3	1.397 (7)
C7—H7	0.9300	B2—F8	1.355 (5)
C8—C9	1.381 (7)	B2—F7	1.363 (5)
C8—H8	0.9300	B2—F6	1.373 (5)
C9—C10	1.372 (6)	B2—F5	1.378 (5)
C9—H9	0.9300		
N3—Cu1—N1	175.88 (14)	C13—C12—H12	120.4
N3—Cu1—O1	92.77 (14)	C11—C12—H12	120.4
N1—Cu1—O1	91.35 (14)	C12—C13—C14	119.1 (4)
N3—Cu1—N4	79.72 (14)	C12—C13—H13	120.4
N1—Cu1—N4	97.76 (14)	C14—C13—H13	120.4
O1—Cu1—N4	129.30 (13)	C15—C14—C13	119.2 (4)
N3—Cu1—N2	98.15 (14)	C15—C14—H14	120.4
N1—Cu1—N2	79.47 (14)	C13—C14—H14	120.4
O1—Cu1—N2	122.65 (14)	N3—C15—C14	121.2 (4)
N4—Cu1—N2	108.05 (13)	N3—C15—C16	114.8 (4)
Cu1—O1—H1A	114.1	C14—C15—C16	124.0 (4)
Cu1—O1—H1B	121.9	N4—C16—C17	121.9 (4)
H1A—O1—H1B	115.8	N4—C16—C15	114.6 (4)
C1—N1—C5	118.3 (4)	C17—C16—C15	123.5 (4)
C1—N1—Cu1	124.3 (3)	C18—C17—C16	119.1 (5)
C5—N1—Cu1	117.3 (3)	C18—C17—H17	120.4
C10—N2—C6	119.3 (4)	C16—C17—H17	120.4
C10—N2—Cu1	128.2 (3)	C17—C18—C19	118.9 (5)
C6—N2—Cu1	112.4 (3)	C17—C18—H18	120.5
C11—N3—C15	118.8 (4)	C19—C18—H18	120.5
C11—N3—Cu1	124.1 (3)	C20—C19—C18	119.6 (5)
C15—N3—Cu1	117.1 (3)	C20—C19—H19	120.2
C16—N4—C20	118.7 (4)	C18—C19—H19	120.2
C16—N4—Cu1	113.4 (3)	N4—C20—C19	121.8 (5)
C20—N4—Cu1	127.7 (3)	N4—C20—H20	119.1
N1—C1—C2	123.1 (5)	C19—C20—H20	119.1
N1—C1—H1	118.4	F3'—B1—F4'	120.7 (10)
C2—C1—H1	118.4	F3'—B1—F4	135.1 (8)
C3—C2—C1	118.5 (5)	F3'—B1—F2	57.0 (6)
C3—C2—H2	120.7	F4'—B1—F2	123.2 (9)
C1—C2—H2	120.7	F4—B1—F2	108.2 (7)
C2—C3—C4	119.0 (4)	F3'—B1—F1	109.6 (9)
C2—C3—H3	120.5	F4'—B1—F1	119.1 (11)
C4—C3—H3	120.5	F4—B1—F1	115.1 (9)
C3—C4—C5	120.5 (4)	F2—B1—F1	111.7 (7)
C3—C4—H4	119.8	F3'—B1—F1'	105.9 (9)
C5—C4—H4	119.8	F4'—B1—F1'	105.6 (12)
N1—C5—C4	120.5 (4)	F4—B1—F1'	112.8 (9)
N1—C5—C6	114.9 (4)	F2—B1—F1'	130.5 (9)
C4—C5—C6	124.6 (4)	F3'—B1—F2'	107.4 (9)
N2—C6—C7	120.6 (4)	F4'—B1—F2'	108.7 (9)
N2—C6—C5	115.9 (4)	F4—B1—F2'	82.0 (7)
C7—C6—C5	123.5 (4)	F2—B1—F2'	52.0 (6)

C8—C7—C6	120.0 (4)	F1—B1—F2'	84.6 (7)
C8—C7—H7	120.0	F1'—B1—F2'	107.9 (9)
C6—C7—H7	120.0	F3'—B1—F3	52.7 (6)
C7—C8—C9	118.6 (4)	F4'—B1—F3	76.6 (8)
C7—C8—H8	120.7	F4—B1—F3	102.0 (7)
C9—C8—H8	120.7	F2—B1—F3	104.2 (7)
C10—C9—C8	118.9 (5)	F1—B1—F3	114.6 (8)
C10—C9—H9	120.6	F1'—B1—F3	93.4 (8)
C8—C9—H9	120.6	F2'—B1—F3	155.1 (9)
N2—C10—C9	122.6 (4)	F8—B2—F7	111.5 (4)
N2—C10—H10	118.7	F8—B2—F6	107.0 (4)
C9—C10—H10	118.7	F7—B2—F6	108.6 (4)
N3—C11—C12	122.5 (4)	F8—B2—F5	109.4 (4)
N3—C11—H11	118.7	F7—B2—F5	110.5 (4)
C12—C11—H11	118.7	F6—B2—F5	109.7 (4)
C13—C12—C11	119.2 (4)		
O1—Cu1—N1—C1	−55.2 (4)	Cu1—N2—C6—C7	176.4 (3)
N4—Cu1—N1—C1	74.8 (4)	C10—N2—C6—C5	−179.2 (4)
N2—Cu1—N1—C1	−178.2 (4)	Cu1—N2—C6—C5	−2.7 (4)
O1—Cu1—N1—C5	122.5 (3)	N1—C5—C6—N2	2.4 (5)
N4—Cu1—N1—C5	−107.5 (3)	C4—C5—C6—N2	−178.8 (4)
N2—Cu1—N1—C5	−0.5 (3)	N1—C5—C6—C7	−176.6 (4)
N3—Cu1—N2—C10	−5.5 (4)	C4—C5—C6—C7	2.2 (7)
N1—Cu1—N2—C10	177.9 (4)	N2—C6—C7—C8	−1.3 (6)
O1—Cu1—N2—C10	93.1 (4)	C5—C6—C7—C8	177.6 (4)
N4—Cu1—N2—C10	−87.3 (4)	C6—C7—C8—C9	1.5 (7)
N3—Cu1—N2—C6	178.3 (3)	C7—C8—C9—C10	−0.3 (7)
N1—Cu1—N2—C6	1.8 (3)	C6—N2—C10—C9	1.5 (6)
O1—Cu1—N2—C6	−83.0 (3)	Cu1—N2—C10—C9	−174.4 (3)
N4—Cu1—N2—C6	96.6 (3)	C8—C9—C10—N2	−1.3 (7)
O1—Cu1—N3—C11	−52.2 (4)	C15—N3—C11—C12	0.4 (7)
N4—Cu1—N3—C11	178.4 (4)	Cu1—N3—C11—C12	179.5 (3)
N2—Cu1—N3—C11	71.4 (4)	N3—C11—C12—C13	0.7 (7)
O1—Cu1—N3—C15	127.0 (3)	C11—C12—C13—C14	−1.5 (7)
N4—Cu1—N3—C15	−2.5 (3)	C12—C13—C14—C15	1.2 (7)
N2—Cu1—N3—C15	−109.5 (3)	C11—N3—C15—C14	−0.7 (6)
N3—Cu1—N4—C16	5.4 (3)	Cu1—N3—C15—C14	−179.9 (3)
N1—Cu1—N4—C16	−177.9 (3)	C11—N3—C15—C16	178.7 (4)
O1—Cu1—N4—C16	−79.8 (3)	Cu1—N3—C15—C16	−0.5 (4)
N2—Cu1—N4—C16	100.7 (3)	C13—C14—C15—N3	−0.1 (6)
N3—Cu1—N4—C20	179.4 (4)	C13—C14—C15—C16	−179.4 (4)
N1—Cu1—N4—C20	−3.9 (4)	C20—N4—C16—C17	−1.6 (6)
O1—Cu1—N4—C20	94.3 (4)	Cu1—N4—C16—C17	173.0 (3)
N2—Cu1—N4—C20	−85.3 (4)	C20—N4—C16—C15	178.3 (4)
C5—N1—C1—C2	1.1 (7)	Cu1—N4—C16—C15	−7.1 (4)
Cu1—N1—C1—C2	178.8 (4)	N3—C15—C16—N4	5.2 (5)
N1—C1—C2—C3	0.3 (8)	C14—C15—C16—N4	−175.4 (4)
C1—C2—C3—C4	−1.0 (8)	N3—C15—C16—C17	−174.8 (4)
C2—C3—C4—C5	0.2 (7)	C14—C15—C16—C17	4.5 (6)

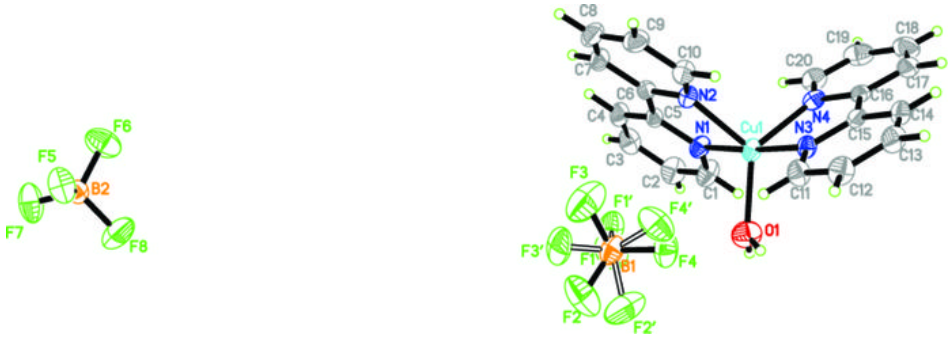
C1—N1—C5—C4	−1.9 (6)	N4—C16—C17—C18	0.1 (6)
Cu1—N1—C5—C4	−179.7 (3)	C15—C16—C17—C18	−179.9 (4)
C1—N1—C5—C6	177.0 (4)	C16—C17—C18—C19	0.9 (7)
Cu1—N1—C5—C6	−0.8 (5)	C17—C18—C19—C20	−0.2 (8)
C3—C4—C5—N1	1.2 (7)	C16—N4—C20—C19	2.3 (6)
C3—C4—C5—C6	−177.5 (4)	Cu1—N4—C20—C19	−171.4 (3)
C10—N2—C6—C7	−0.2 (6)	C18—C19—C20—N4	−1.4 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···F8^{i}	0.86	2.26	3.113 (4)	171
O1—H1B···F7^{ii}	0.86	2.44	3.038 (4)	127

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

Fig. 1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