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

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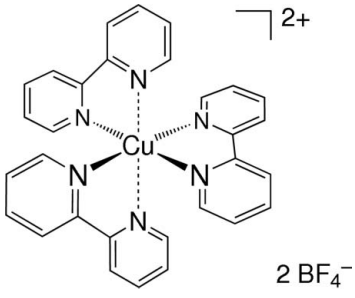
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.036; wR factor = 0.088; data-to-parameter ratio = 13.6.

The title compound, $[Cu(C_{10}H_8N_2)_3](BF_4)_2$, shows the expected Jahn–Teller distortion at the pseudo-octahedrally coordinated Cu^{II} atom. Each Cu^{II} complex cation is surrounded by six BF_4^- anions and each anion by three cations with weak C—H···F hydrogen bonds between them. One of the two BF_4^- anions exhibits a rotational disorder (0.6:0.4) around one of the B—F bonds.

Related literature

For related literature, see: Althoff *et al.* (2006); Anderson (1972); Dong *et al.* (2006); Faulmann *et al.* (1998); Janiak *et al.* (1999); Janiak (2000); Juric *et al.* (2006); Liu *et al.* (1991); Majumdar *et al.* (1998); Murphy *et al.* (2006); Nishio (2004); Niu *et al.* (2004); Pavlishchuk *et al.* (1999); Perkins *et al.* (2006); van Albada *et al.* (2004); Yang *et al.* (2004*a*,*b*); Wu *et al.* (2003).



Experimental

Crystal data

$[Cu(C_{10}H_8N_2)_3](BF_4)_2$
M_r = 705.72
Triclinic, $P\overline{1}$
a = 7.8633 (2) Å
b = 10.7810 (2) Å
c = 18.3211 (4) Å
α = 101.118 (1)°
β = 90.750 (1)°
γ = 98.091 (1)°
V = 1507.54 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 203 (2) K
0.29 × 0.09 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.799, T_{max} = 0.955
35533 measured reflections
6145 independent reflections
4809 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.088
S = 1.06
6145 reflections
451 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N4	2.0144 (16)	Cu—N1	2.0347 (15)
Cu—N2	2.0309 (16)	Cu—N3	2.2388 (16)
Cu—N6	2.0313 (16)	Cu—N5	2.4506 (16)
N4—Cu—N2	174.08 (6)	N6—Cu—N3	101.71 (6)
N4—Cu—N6	91.04 (6)	N1—Cu—N3	91.97 (6)
N2—Cu—N6	94.81 (6)	N4—Cu—N5	99.13 (6)
N4—Cu—N1	94.04 (6)	N2—Cu—N5	83.42 (6)
N2—Cu—N1	80.47 (6)	N6—Cu—N5	74.14 (6)
N6—Cu—N1	166.16 (6)	N1—Cu—N5	92.33 (6)
N4—Cu—N3	77.31 (7)	N3—Cu—N5	174.61 (6)
N2—Cu—N3	100.51 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···F2^{i}	0.94	2.54	3.342 (3)	144
C8—H8A···F2^{ii}	0.94	2.35	3.274 (3)	169
C10—H10A···F6B^{iii}	0.94	2.49	3.376 (4)	158
C13—H13A···F8B^{iv}	0.94	2.17	3.063 (5)	158
C26—H26A···F4	0.94	2.31	3.191 (3)	155
C27—H27A···F1	0.94	2.54	3.303 (3)	138

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2177).

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supplementary materials

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

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Comment

Metal complexes with three (modified) 2,2'-bipyridine ligands are of continous interest (Janiak *et al.*, 1999; Wu *et al.*, 2003; Yang *et al.*, 2004*a*,b). Tris(2,2'-bipyridine)copper structure are known with the anions tris(oxalato)chromate(III) (Juric *et al.*, 2006), polyoxovanadate (Dong *et al.*, 2006), polyoxotungstate (Niu *et al.*, 2004), bis(bis(2-thioxo-1,3-dithiole-4,5-dithiolato)- nickelate(II) (Faulmann *et al.*, 1998), tetraphenylborate (Murphy *et al.*, 2006) and perchlorate (Anderson, 1972; Liu *et al.*, 1991; Majumdar *et al.*, 1998; Pavlishchuk *et al.*, 1999). The closely related tris(5,5'-dimethyl-2,2'-bipyridine)copper(II) complexes have been reported as the hexafluorophosphate (Perkins *et al.*, 2006) and tetrafluoroborate salt (van Albada *et al.*, 2004).

The asymmetric unit of the title complex is shown in Fig. 1. The cation-anion packing view projected onto the *bc* plane is given in Fig. 2. Bond lengths and angles in the title complex (Table 1) are as expected from the related $[Cu(2,2'\text{-bipy})_3]$-compounds with other anions. The crystal packing is primarily governed by the electrostatic cation-anion interaction and separation. Some weak C—H···F interactions from the bipyridine to the BF_4-anion can be discerned (Althoff *et al.*, 2006). No relevant π—π or C—H···π interactions were found (Janiak, 2000; Nishio, 2004).

Noteworthy, the long Cu···N5 distortion apparently leads to a sizable tilt angle between the pyridyl ring planes of N5 and N6 of 32.1 (1)°, while the other two ring planes show tilt angles of 14.5 (1)° (N1,N2) or 11.0 (1)° (N3,N4).

Experimental

A methanol solution (30 ml) of $Cu(BF_4)_2{\cdot}6H_2O$ (5 mmol, 1.726 g) was mixed with *L*-glutamic acid (5 mmol, 0.781 g) and the mixture was warmed on a water bath for 5 minutes. The resulting blue solution was added to a methanol solution (10 ml) of 2,2'-bipyridine (5 mmol, 0.780 g). The dark blue solution was stirred for 15 min. Blue crystals were obtained by slow evaporation of the mother liquor after two days. The crystals were analyzed as the title compound. For a direct preparation an aqueous solution (10 ml) of $Cu(BF_4)_2{\cdot}6H_2O$ (2 mmol, 0.690 g) was mixed with a methanol solution (5 ml) of 2,2'-bipyridine (6 mmol, 0.937 g) and the mixture was refluxed for approximately 2 h. After two days at room temperature long light blue crystals were obtained (yield 68%). Analysis calculated for $C_{30}H_{24}CuB_2F_8N_6$ (705.72): C 51.06, H 3.43, N 11.91%; found: C 51.30, H, 3.15, N 11.73%.

Refinement

H atoms were positioned geometrically (C—H = 0.94 Å) and refined using a riding model (AFIX 43), with $U_{iso}(H) = 1.2U_{eq}(C)$. The disordered F atoms on B2 were refined anisotropically by assigning them to different PART numbers of a disordered group. The atoms of PART 1 (F6A, F7A and F8) were found to have an occupation factor (sof) of 0.4. The atoms of PART 2 (F6B, F7B, F8B) had an occupation factor of 0.6. These occupation factors were initially found upon refinement and then fixed in subsequent refinement cycles.

Figures

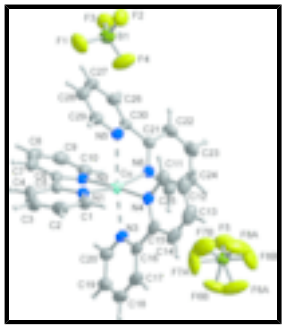


Fig. 1. : Asymmetric unit of $[Cu(2,2'\text{-bipy})_3](BF_4)_2$, also showing the rotational disorder of one BF_4 anion.

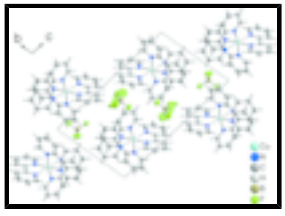


Fig. 2. : Crystal packing projected onto the *bc* plane, illustrating the cation-anion separation.

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

Crystal data

$[Cu(C_{10}H_8N_2)_3](BF_4)_2$	$Z = 2$
$M_r = 705.72$	$F_{000} = 714$
Triclinic, $P\overline{1}$	$D_x = 1.555$ Mg m^{-3}
$a = 7.8633$ (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.7810$ (2) Å	Cell parameters from 9932 reflections
$c = 18.3211$ (4) Å	$\theta = 4.9$–57.9°
$\alpha = 101.118$ (1)°	$\mu = 0.81$ mm^{-1}
$\beta = 90.750$ (1)°	$T = 203$ (2) K
$\gamma = 98.091$ (1)°	Needle, blue
$V = 1507.54$ (6) Å^3	0.29 × 0.09 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer	6145 independent reflections
Radiation source: fine-focus sealed tube	4809 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.081$
$T = 203$(2) K	$\theta_{max} = 26.4^\circ$
ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.799$, $T_{max} = 0.955$	$k = -13 \rightarrow 13$
35533 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.2354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
6145 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
451 parameters	$\Delta\rho_{min} = -0.30$ 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}	Occ. (<1)
Cu	0.49641 (3)	0.26662 (2)	0.259958 (10)	0.02981 (9)	
N1	0.6154 (2)	0.14377 (15)	0.18640 (7)	0.0324 (4)	
N2	0.6720 (2)	0.39431 (15)	0.22253 (7)	0.0323 (4)	
N3	0.6455 (2)	0.23049 (16)	0.35676 (8)	0.0362 (4)	
N4	0.3385 (2)	0.12645 (15)	0.29363 (8)	0.0351 (4)	
N5	0.3100 (2)	0.30720 (16)	0.16155 (8)	0.0356 (4)	
N6	0.3548 (2)	0.39973 (15)	0.31069 (7)	0.0317 (4)	
C1	0.5892 (3)	0.0164 (2)	0.17581 (10)	0.0410 (5)	
H1A	0.5004	−0.0236	0.2009	0.049*	
C2	0.6876 (3)	−0.0589 (2)	0.12940 (11)	0.0506 (6)	
H2A	0.6664	−0.1484	0.1233	0.061*	
C3	0.8163 (3)	−0.0012 (3)	0.09252 (12)	0.0569 (7)	
H3A	0.8854	−0.0507	0.0610	0.068*	
C4	0.8438 (3)	0.1303 (2)	0.10199 (11)	0.0507 (6)	
H4A	0.9316	0.1713	0.0769	0.061*	
C5	0.7400 (3)	0.2015 (2)	0.14913 (9)	0.0354 (5)	
C6	0.7582 (3)	0.3416 (2)	0.16347 (9)	0.0355 (5)	
C7	0.8520 (3)	0.4170 (2)	0.12031 (10)	0.0489 (6)	

H7A	0.9077	0.3790	0.0786	0.059*
C8	0.8627 (3)	0.5479 (3)	0.13910 (12)	0.0543 (6)
H8A	0.9243	0.6002	0.1100	0.065*
C9	0.7822 (3)	0.6010 (2)	0.20101 (12)	0.0489 (6)
H9B	0.7917	0.6903	0.2158	0.059*
C10	0.6867 (3)	0.5218 (2)	0.24154 (11)	0.0397 (5)
H10A	0.6307	0.5587	0.2835	0.048*
C11	0.1779 (3)	0.0876 (2)	0.26544 (11)	0.0454 (5)
H11A	0.1367	0.1283	0.2292	0.055*
C12	0.0703 (3)	−0.0097 (2)	0.28738 (12)	0.0560 (6)
H12A	−0.0427	−0.0343	0.2671	0.067*
C13	0.1320 (4)	−0.0700 (2)	0.33951 (13)	0.0621 (7)
H13A	0.0619	−0.1370	0.3554	0.074*
C14	0.2974 (4)	−0.0314 (2)	0.36820 (11)	0.0552 (7)
H14A	0.3413	−0.0731	0.4033	0.066*
C15	0.3999 (3)	0.06876 (18)	0.34562 (9)	0.0391 (5)
C16	0.5772 (3)	0.12056 (19)	0.37568 (9)	0.0390 (5)
C17	0.6688 (4)	0.0604 (2)	0.42061 (11)	0.0513 (6)
H17A	0.6200	−0.0173	0.4329	0.062*
C18	0.8314 (4)	0.1164 (3)	0.44662 (12)	0.0572 (7)
H18A	0.8949	0.0773	0.4771	0.069*
C19	0.9016 (3)	0.2303 (2)	0.42800 (11)	0.0515 (6)
H19A	1.0126	0.2701	0.4455	0.062*
C20	0.8033 (3)	0.2841 (2)	0.38278 (10)	0.0436 (5)
H20A	0.8499	0.3617	0.3698	0.052*
C21	0.2698 (3)	0.46343 (18)	0.26934 (9)	0.0335 (4)
C22	0.1715 (3)	0.5548 (2)	0.30129 (11)	0.0462 (5)
H22A	0.1144	0.5991	0.2715	0.055*
C23	0.1587 (3)	0.5800 (2)	0.37805 (11)	0.0517 (6)
H23A	0.0922	0.6414	0.4009	0.062*
C24	0.2440 (3)	0.5144 (2)	0.42011 (10)	0.0449 (5)
H24A	0.2360	0.5298	0.4721	0.054*
C25	0.3416 (3)	0.4256 (2)	0.38535 (9)	0.0375 (5)
H25A	0.4010	0.3816	0.4145	0.045*
C26	0.2875 (3)	0.5179 (2)	0.14170 (10)	0.0401 (5)
H26A	0.2726	0.6026	0.1616	0.048*
C27	0.3104 (3)	0.4783 (2)	0.06585 (11)	0.0462 (5)
H27A	0.3122	0.5363	0.0335	0.055*
C28	0.3300 (3)	0.3536 (2)	0.03931 (10)	0.0454 (5)
H28A	0.3433	0.3246	−0.0118	0.054*
C29	0.3300 (3)	0.2709 (2)	0.08831 (10)	0.0405 (5)
H29A	0.3447	0.1857	0.0695	0.049*
C30	0.2876 (2)	0.42833 (19)	0.18674 (9)	0.0321 (4)
B1	0.2109 (4)	0.8267 (2)	0.08406 (13)	0.0473 (6)
F1	0.3396 (2)	0.77651 (16)	0.04220 (9)	0.0756 (5)
F2	0.05285 (19)	0.76224 (13)	0.05089 (7)	0.0608 (4)
F3	0.21961 (19)	0.95517 (12)	0.08408 (7)	0.0577 (4)
F4	0.2248 (3)	0.80748 (14)	0.15576 (7)	0.0805 (5)
B2	0.3042 (3)	0.2767 (2)	0.57012 (12)	0.0416 (6)

F5	0.2891 (2)	0.40217 (15)	0.57208 (9)	0.0755 (5)	
F6A	0.3457 (11)	0.2434 (5)	0.6377 (3)	0.103 (3)	0.40
F7A	0.4247 (8)	0.2392 (6)	0.5222 (4)	0.097 (2)	0.40
F8A	0.1552 (8)	0.1886 (6)	0.5459 (4)	0.099 (2)	0.40
F6B	0.4403 (5)	0.2725 (4)	0.6134 (2)	0.0805 (12)	0.60
F7B	0.3161 (7)	0.2142 (5)	0.50027 (17)	0.1027 (16)	0.60
F8B	0.1604 (5)	0.2332 (4)	0.5983 (3)	0.1105 (16)	0.60

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.03426 (15)	0.02520 (13)	0.03177 (11)	0.00620 (10)	0.00703 (9)	0.00832 (8)
N1	0.0350 (10)	0.0322 (9)	0.0305 (6)	0.0084 (7)	0.0020 (6)	0.0053 (6)
N2	0.0315 (9)	0.0327 (9)	0.0338 (7)	0.0015 (7)	−0.0009 (6)	0.0116 (6)
N3	0.0471 (11)	0.0314 (9)	0.0332 (7)	0.0103 (8)	0.0042 (7)	0.0108 (6)
N4	0.0413 (11)	0.0275 (9)	0.0374 (7)	0.0060 (8)	0.0106 (7)	0.0073 (6)
N5	0.0382 (10)	0.0329 (9)	0.0358 (7)	0.0054 (8)	−0.0022 (7)	0.0072 (6)
N6	0.0346 (9)	0.0276 (9)	0.0333 (7)	0.0062 (7)	0.0036 (6)	0.0060 (6)
C1	0.0488 (14)	0.0369 (12)	0.0385 (9)	0.0126 (10)	0.0031 (9)	0.0057 (8)
C2	0.0652 (17)	0.0406 (13)	0.0471 (10)	0.0237 (12)	−0.0017 (11)	0.0003 (9)
C3	0.0567 (16)	0.0674 (18)	0.0480 (11)	0.0321 (14)	0.0063 (11)	−0.0022 (11)
C4	0.0393 (13)	0.0699 (17)	0.0436 (10)	0.0148 (12)	0.0114 (9)	0.0076 (10)
C5	0.0298 (11)	0.0486 (12)	0.0296 (7)	0.0096 (9)	−0.0003 (7)	0.0090 (8)
C6	0.0272 (11)	0.0484 (13)	0.0314 (8)	0.0016 (9)	−0.0012 (7)	0.0122 (8)
C7	0.0403 (13)	0.0667 (16)	0.0397 (9)	−0.0062 (12)	0.0034 (9)	0.0204 (10)
C8	0.0478 (15)	0.0636 (17)	0.0539 (11)	−0.0126 (12)	−0.0048 (10)	0.0330 (11)
C9	0.0442 (14)	0.0379 (12)	0.0645 (12)	−0.0063 (11)	−0.0150 (11)	0.0199 (10)
C10	0.0373 (12)	0.0354 (12)	0.0470 (9)	0.0006 (9)	−0.0055 (9)	0.0132 (8)
C11	0.0485 (14)	0.0379 (12)	0.0482 (10)	0.0035 (11)	0.0108 (10)	0.0058 (9)
C12	0.0567 (16)	0.0459 (14)	0.0581 (12)	−0.0090 (12)	0.0134 (11)	0.0033 (10)
C13	0.076 (2)	0.0440 (14)	0.0608 (13)	−0.0149 (13)	0.0203 (13)	0.0121 (11)
C14	0.082 (2)	0.0408 (13)	0.0459 (10)	0.0038 (13)	0.0152 (11)	0.0188 (9)
C15	0.0572 (14)	0.0269 (10)	0.0346 (8)	0.0085 (10)	0.0158 (9)	0.0072 (7)
C16	0.0556 (15)	0.0344 (11)	0.0313 (8)	0.0154 (10)	0.0138 (8)	0.0099 (7)
C17	0.0686 (18)	0.0457 (14)	0.0507 (11)	0.0240 (13)	0.0144 (11)	0.0251 (10)
C18	0.0683 (19)	0.0680 (17)	0.0495 (11)	0.0368 (15)	0.0094 (11)	0.0269 (11)
C19	0.0518 (15)	0.0650 (16)	0.0429 (10)	0.0210 (13)	0.0015 (10)	0.0144 (10)
C20	0.0500 (15)	0.0440 (13)	0.0385 (9)	0.0088 (11)	0.0007 (9)	0.0107 (8)
C21	0.0329 (11)	0.0309 (10)	0.0366 (8)	0.0065 (9)	0.0008 (8)	0.0052 (7)
C22	0.0461 (14)	0.0461 (13)	0.0483 (10)	0.0203 (11)	−0.0029 (9)	0.0046 (9)
C23	0.0513 (15)	0.0514 (14)	0.0517 (11)	0.0233 (12)	0.0061 (10)	−0.0036 (10)
C24	0.0497 (14)	0.0462 (13)	0.0372 (9)	0.0125 (11)	0.0082 (9)	0.0004 (9)
C25	0.0398 (12)	0.0376 (11)	0.0355 (8)	0.0053 (9)	0.0045 (8)	0.0082 (8)
C26	0.0428 (13)	0.0332 (11)	0.0464 (9)	0.0099 (10)	−0.0024 (9)	0.0097 (8)
C27	0.0496 (14)	0.0498 (14)	0.0446 (10)	0.0083 (11)	0.0005 (9)	0.0216 (9)
C28	0.0494 (14)	0.0519 (14)	0.0344 (8)	0.0071 (11)	−0.0007 (9)	0.0077 (9)
C29	0.0457 (13)	0.0370 (12)	0.0367 (8)	0.0078 (10)	−0.0033 (8)	0.0013 (8)
C30	0.0270 (11)	0.0324 (11)	0.0368 (8)	0.0057 (8)	−0.0022 (7)	0.0062 (7)

B1	0.0596 (18)	0.0304 (13)	0.0518 (12)	0.0077 (12)	−0.0008 (12)	0.0069 (10)
F1	0.0628 (11)	0.0641 (11)	0.0981 (11)	0.0240 (9)	0.0108 (8)	0.0003 (8)
F2	0.0574 (9)	0.0529 (9)	0.0687 (8)	−0.0077 (7)	0.0027 (7)	0.0154 (7)
F3	0.0666 (10)	0.0331 (7)	0.0749 (8)	0.0067 (7)	0.0047 (7)	0.0149 (6)
F4	0.1436 (17)	0.0460 (9)	0.0540 (7)	0.0211 (10)	−0.0122 (9)	0.0108 (6)
B2	0.0395 (15)	0.0437 (15)	0.0414 (10)	0.0055 (12)	−0.0028 (10)	0.0091 (10)
F5	0.0962 (13)	0.0488 (9)	0.0854 (9)	0.0195 (9)	−0.0092 (9)	0.0170 (8)
F6A	0.209 (9)	0.056 (4)	0.047 (2)	0.057 (4)	−0.040 (4)	−0.008 (2)
F7A	0.084 (4)	0.084 (4)	0.116 (5)	0.009 (4)	0.064 (4)	0.003 (4)
F8A	0.075 (4)	0.072 (4)	0.147 (5)	−0.023 (3)	−0.056 (5)	0.046 (4)
F6B	0.064 (2)	0.063 (2)	0.114 (3)	0.0096 (17)	−0.045 (2)	0.021 (2)
F7B	0.159 (5)	0.103 (3)	0.0495 (14)	0.061 (4)	0.004 (2)	−0.0062 (16)
F8B	0.051 (2)	0.096 (3)	0.206 (5)	0.010 (2)	0.051 (3)	0.079 (3)

Geometric parameters (Å, °)

Cu—N4	2.0144 (16)	C13—H13A	0.9400
Cu—N2	2.0309 (16)	C14—C15	1.387 (3)
Cu—N6	2.0313 (16)	C14—H14A	0.9400
Cu—N1	2.0347 (15)	C15—C16	1.483 (3)
Cu—N3	2.2388 (16)	C16—C17	1.392 (3)
Cu—N5	2.4506 (16)	C17—C18	1.372 (4)
N1—C1	1.335 (3)	C17—H17A	0.9400
N1—C5	1.350 (2)	C18—C19	1.380 (3)
N2—C10	1.339 (3)	C18—H18A	0.9400
N2—C6	1.358 (2)	C19—C20	1.383 (3)
N3—C20	1.333 (3)	C19—H19A	0.9400
N3—C16	1.341 (3)	C20—H20A	0.9400
N4—C11	1.337 (3)	C21—C22	1.383 (3)
N4—C15	1.352 (3)	C21—C30	1.501 (2)
N5—C30	1.336 (2)	C22—C23	1.388 (3)
N5—C29	1.341 (2)	C22—H22A	0.9400
N6—C21	1.345 (3)	C23—C24	1.369 (3)
N6—C25	1.351 (2)	C23—H23A	0.9400
C1—C2	1.381 (3)	C24—C25	1.377 (3)
C1—H1A	0.9400	C24—H24A	0.9400
C2—C3	1.368 (4)	C25—H25A	0.9400
C2—H2A	0.9400	C26—C30	1.386 (3)
C3—C4	1.380 (4)	C26—C27	1.395 (3)
C3—H3A	0.9400	C26—H26A	0.9400
C4—C5	1.393 (3)	C27—C28	1.370 (3)
C4—H4A	0.9400	C27—H27A	0.9400
C5—C6	1.468 (3)	C28—C29	1.382 (3)
C6—C7	1.387 (3)	C28—H28A	0.9400
C7—C8	1.377 (3)	C29—H29A	0.9400
C7—H7A	0.9400	B1—F4	1.374 (3)
C8—C9	1.373 (3)	B1—F3	1.377 (3)
C8—H8A	0.9400	B1—F1	1.386 (3)
C9—C10	1.387 (3)	B1—F2	1.404 (3)

C9—H9B	0.9400	B2—F8B	1.313 (4)
C10—H10A	0.9400	B2—F6B	1.334 (4)
C11—C12	1.379 (3)	B2—F7B	1.337 (4)
C11—H11A	0.9400	B2—F7A	1.351 (5)
C12—C13	1.373 (4)	B2—F5	1.368 (3)
C12—H12A	0.9400	B2—F6A	1.402 (5)
C13—C14	1.373 (4)	B2—F8A	1.409 (6)
N4—Cu—N2	174.08 (6)	C12—C13—H13A	120.3
N4—Cu—N6	91.04 (6)	C13—C14—C15	120.3 (2)
N2—Cu—N6	94.81 (6)	C13—C14—H14A	119.8
N4—Cu—N1	94.04 (6)	C15—C14—H14A	119.8
N2—Cu—N1	80.47 (6)	N4—C15—C14	119.9 (2)
N6—Cu—N1	166.16 (6)	N4—C15—C16	115.94 (17)
N4—Cu—N3	77.31 (7)	C14—C15—C16	124.2 (2)
N2—Cu—N3	100.51 (6)	N3—C16—C17	121.4 (2)
N6—Cu—N3	101.71 (6)	N3—C16—C15	115.58 (18)
N1—Cu—N3	91.97 (6)	C17—C16—C15	123.0 (2)
N4—Cu—N5	99.13 (6)	C18—C17—C16	118.8 (2)
N2—Cu—N5	83.42 (6)	C18—C17—H17A	120.6
N6—Cu—N5	74.14 (6)	C16—C17—H17A	120.6
N1—Cu—N5	92.33 (6)	C17—C18—C19	120.0 (2)
N3—Cu—N5	174.61 (6)	C17—C18—H18A	120.0
C1—N1—C5	119.01 (17)	C19—C18—H18A	120.0
C1—N1—Cu	126.67 (13)	C18—C19—C20	117.9 (2)
C5—N1—Cu	114.18 (13)	C18—C19—H19A	121.0
C10—N2—C6	118.84 (17)	C20—C19—H19A	121.0
C10—N2—Cu	126.24 (13)	N3—C20—C19	122.8 (2)
C6—N2—Cu	113.80 (13)	N3—C20—H20A	118.6
C20—N3—C16	119.03 (18)	C19—C20—H20A	118.6
C20—N3—Cu	128.30 (13)	N6—C21—C22	121.80 (16)
C16—N3—Cu	110.50 (13)	N6—C21—C30	115.75 (17)
C11—N4—C15	119.49 (18)	C22—C21—C30	122.44 (18)
C11—N4—Cu	122.36 (14)	C21—C22—C23	119.0 (2)
C15—N4—Cu	118.14 (14)	C21—C22—H22A	120.5
C30—N5—C29	117.54 (18)	C23—C22—H22A	120.5
C30—N5—Cu	102.31 (11)	C24—C23—C22	119.2 (2)
C29—N5—Cu	124.94 (14)	C24—C23—H23A	120.4
C21—N6—C25	118.56 (17)	C22—C23—H23A	120.4
C21—N6—Cu	119.66 (11)	C23—C24—C25	119.25 (18)
C25—N6—Cu	121.77 (14)	C23—C24—H24A	120.4
N1—C1—C2	122.5 (2)	C25—C24—H24A	120.4
N1—C1—H1A	118.8	N6—C25—C24	122.2 (2)
C2—C1—H1A	118.8	N6—C25—H25A	118.9
C3—C2—C1	119.0 (2)	C24—C25—H25A	118.9
C3—C2—H2A	120.5	C30—C26—C27	117.9 (2)
C1—C2—H2A	120.5	C30—C26—H26A	121.1
C2—C3—C4	119.4 (2)	C27—C26—H26A	121.1
C2—C3—H3A	120.3	C28—C27—C26	118.9 (2)
C4—C3—H3A	120.3	C28—C27—H27A	120.5

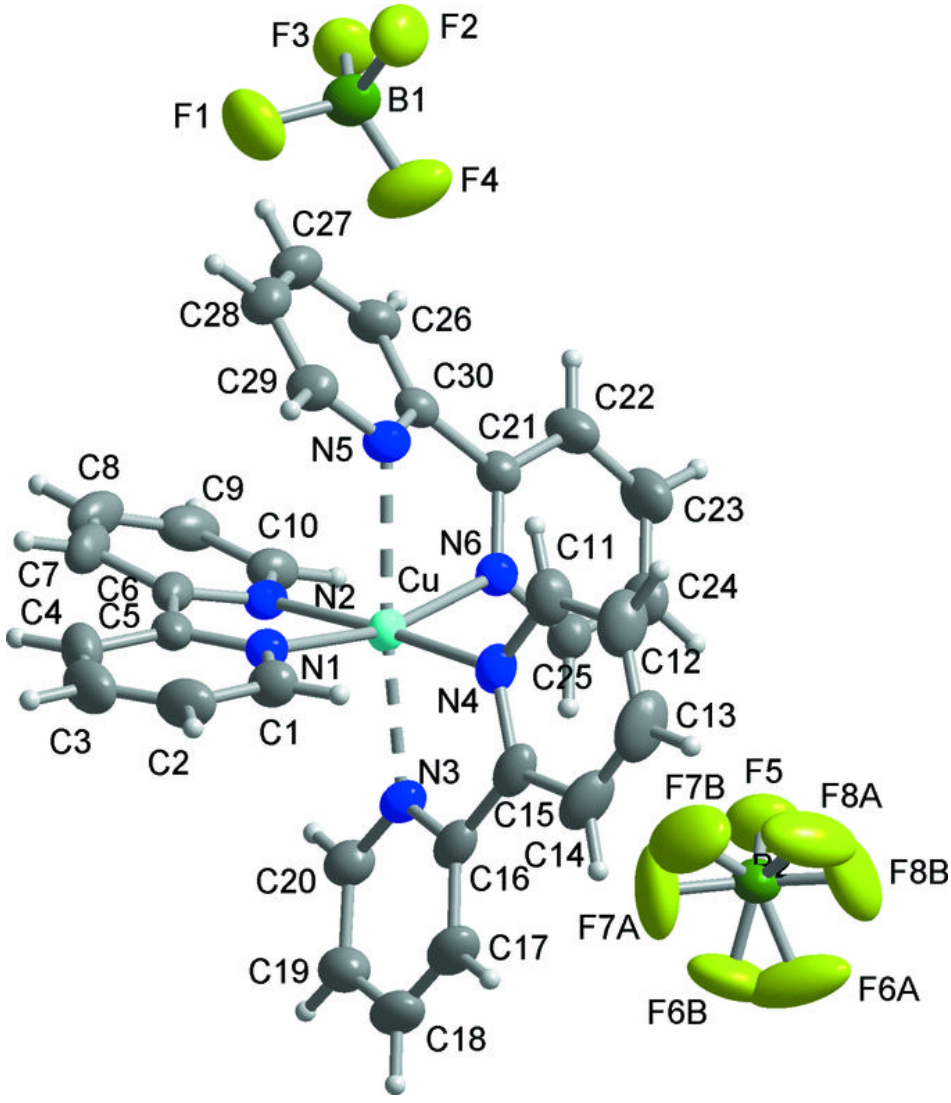
C3—C4—C5	119.2 (2)	C26—C27—H27A	120.5
C3—C4—H4A	120.4	C27—C28—C29	119.40 (18)
C5—C4—H4A	120.4	C27—C28—H28A	120.3
N1—C5—C4	120.9 (2)	C29—C28—H28A	120.3
N1—C5—C6	115.26 (16)	N5—C29—C28	122.7 (2)
C4—C5—C6	123.83 (19)	N5—C29—H29A	118.7
N2—C6—C7	121.2 (2)	C28—C29—H29A	118.7
N2—C6—C5	114.73 (16)	N5—C30—C26	123.60 (16)
C7—C6—C5	124.03 (18)	N5—C30—C21	114.84 (17)
C8—C7—C6	119.5 (2)	C26—C30—C21	121.51 (18)
C8—C7—H7A	120.3	F4—B1—F3	110.12 (18)
C6—C7—H7A	120.3	F4—B1—F1	110.1 (2)
C9—C8—C7	119.1 (2)	F3—B1—F1	110.5 (2)
C9—C8—H8A	120.5	F4—B1—F2	109.4 (2)
C7—C8—H8A	120.5	F3—B1—F2	109.2 (2)
C8—C9—C10	119.4 (2)	F1—B1—F2	107.39 (18)
C8—C9—H9B	120.3	F8B—B2—F6B	111.3 (3)
C10—C9—H9B	120.3	F8B—B2—F7B	110.6 (4)
N2—C10—C9	121.8 (2)	F6B—B2—F7B	112.2 (3)
N2—C10—H10A	119.1	F8B—B2—F5	103.0 (3)
C9—C10—H10A	119.1	F6B—B2—F5	108.2 (3)
N4—C11—C12	122.6 (2)	F7B—B2—F5	111.2 (3)
N4—C11—H11A	118.7	F7A—B2—F5	110.5 (4)
C12—C11—H11A	118.7	F7A—B2—F6A	106.7 (5)
C13—C12—C11	118.4 (2)	F5—B2—F6A	116.9 (3)
C13—C12—H12A	120.8	F7A—B2—F8A	104.6 (4)
C11—C12—H12A	120.8	F5—B2—F8A	115.6 (3)
C14—C13—C12	119.3 (2)	F6A—B2—F8A	101.4 (4)
C14—C13—H13A	120.3		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3A···F2^{i}	0.94	2.54	3.342 (3)	144
C8—H8A···F2^{ii}	0.94	2.35	3.274 (3)	169
C10—H10A···F6B^{iii}	0.94	2.49	3.376 (4)	158
C13—H13A···F8B^{iv}	0.94	2.17	3.063 (5)	158
C26—H26A···F4	0.94	2.31	3.191 (3)	155
C27—H27A···F1	0.94	2.54	3.303 (3)	138

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

Fig. 1


F3
F2
F1
B1
F4
C27
C28
C26
C29
C30
C22
N5
C21
C8
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C10
N6
C11
C7
C6
Cu
C24
C4
C5
N2
N1
C25
C12
N4
C13
C3
C2
C1
N3
F7B
F5
F8A
C15
C14
F8B
C20
C16
F7A
C17
C19
F6A
F6B
C18

Fig. 2