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

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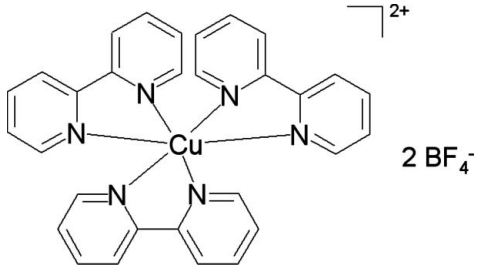
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.061; wR factor = 0.160; data-to-parameter ratio = 11.7.

The Cu atom in the title salt, $[Cu(C_{10}H_8N_2)_3](BF_4)_2$, has an elongated octahedral coordination geometry. Three F atoms of one anion are disordered over two positions with a site occupancy ratio of 3:2.

Related literature

For the diperchlorate salt, see Anderson (1972), Liu *et al.* (1991), Majumdar *et al.* (1998) and Pavlishchuk *et al.* (1999). For the bis(tetraphenylborate) salt, see Murphy *et al.* (2006), and for the bis(hexafluoridophosphate) salt, see Wang *et al.* (2007).



Experimental

Crystal data

$[Cu(C_{10}H_8N_2)_3](BF_4)_2$
M_r = 705.71
Triclinic, $P\overline{1}$
a = 7.911 (2) Å
b = 10.851 (2) Å
c = 18.482 (4) Å
α = 100.88 (3)°
β = 90.26 (2)°
γ = 98.08 (3)°
V = 1541.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 291 (2) K
0.20 × 0.12 × 0.10 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.858, T_{max} = 0.925
13060 measured reflections
5276 independent reflections
4853 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.160
S = 1.07
5276 reflections
452 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.019 (3)	Cu1—N5	2.044 (3)
Cu1—N6	2.032 (3)	Cu1—N1	2.239 (3)
Cu1—N3	2.034 (3)	Cu1—N4	2.445 (3)
N2—Cu1—N6	94.42 (11)	N3—Cu1—N1	101.62 (11)
N2—Cu1—N3	91.40 (11)	N5—Cu1—N1	99.84 (11)
N6—Cu1—N3	165.91 (11)	N2—Cu1—N4	99.54 (12)
N2—Cu1—N5	173.96 (11)	N6—Cu1—N4	92.01 (10)
N6—Cu1—N5	80.24 (11)	N3—Cu1—N4	74.35 (10)
N3—Cu1—N5	94.44 (11)	N5—Cu1—N4	83.56 (10)
N2—Cu1—N1	77.41 (12)	N1—Cu1—N4	175.00 (10)
N6—Cu1—N1	92.18 (11)		

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2000); 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: NG2301).

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supplementary materials

Acta Cryst. (2007). E**63**, m2254 [**doi:10.1107/S1600536807037002**]

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

W. Huang

Comment

The crystal structure of tris(2,2'-bipyridine)copper diperchlorate (Anderson, 1972; Liu *et al.*, 1991; Majumdar *et al.*, 1998; Pavlishchuk *et al.*, 1999) and tris(2,2'-bipyridine)copper bis(tetraphenylborate) (Murphy *et al.*, 2006) have been reported previously. We have reported the bis(hexafluoridophosphorate) salt (Wang *et al.*, 2007), and continue our work with the bis(tetrafluoridoborate) salt.

The geometry of the copper atom is an elongated octahedron as the structure has four nearly identical Cu–N bonds and two somewhat longer ones that are *trans* to each other. The three 2,2'-bipyridine rings are bent, with dihedral angles of 11.2 (3)° (between C1 to C5 and N1 ring and C6 to C10 N2 ring), 31.0 (3)° (between C11 to C15 and N3 ring and C16 to C20 N4 ring) and 14.6 (3)° (between C21 to C25 and N5 ring and C26 to C30 N6 ring).

Experimental

The compound was obtained by refluxing $Cu(NO_3)_2{\cdot}3H_2O$ (0.121 g, 0.5 mmol) and 2,2'-bipyridine (0.234 g, 1.5 mmol) in a mixture of 80 ml e thanol and 20 ml water for 1 h in the presence of excess $NaBF_4$. The mixture was concentrated to nearly 5 ml. The blue product was recrystallized from a 3/1 methanol water mixture and the pure compound isolated in 90% yield. CH&N elemental analysis. Calculated for $C_{30}H_{24}CuN_6F_{12}P_2$: C 51.06, H 3.43, N 11.91%; found: C 51.04, H 3.49, N 11.86%.

Refinement

The non-hydrogen atoms were refined anisotropically, whereas the H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and refined as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C). F5, F6 and F7 atoms of one tetrafluoridoborate anion are refined over two sites with 0.60 (2): 0.40 (2) site occupancy factors.

Figures

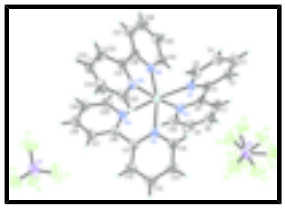


Fig. 1. Molecular plot, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and the H atoms are shown as small spheres of arbitrary radii.

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

Crystal data

$[Cu(C_{10}H_8N_2)_3](BF_4)_2$	$Z = 2$
$M_r = 705.71$	$F_{000} = 714$
Triclinic, $P\overline{1}$	$D_x = 1.521$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.911$ (2) Å	Cell parameters from 6691 reflections
$b = 10.851$ (2) Å	$\theta = 3.0$–$27.5°$
$c = 18.482$ (4) Å	$\mu = 0.79$ mm^{-1}
$\alpha = 100.88$ (3)°	$T = 291$ (2) K
$\beta = 90.26$ (2)°	Block, blue
$\gamma = 98.08$ (3)°	0.20 × 0.12 × 0.10 mm
$V = 1541.8$ (6) Å^3	

Data collection

Rigaku Mercury CCD area-detector diffractometer	5276 independent reflections
Radiation source: Rigaku rotating anode	4853 reflections with $I > 2\sigma(I)$
Monochromator: graphite monochromator	$R_{int} = 0.095$
Detector resolution: 14.6199 pixels mm^{-1}	$\theta_{max} = 25.0°$
$T = 291(2)$ K	$\theta_{min} = 3.0°$
φ and ω scans	$h = -9\rightarrow9$
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	$k = -12\rightarrow11$
$T_{min} = 0.858$, $T_{max} = 0.925$	$l = -21\rightarrow20$
13060 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.160$	$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2 + 0.8259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
5276 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
452 parameters	$\Delta\rho_{min} = -0.77$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The structure was solved by direct methods (Bruker, 2000) and successive difference Fourier syntheses.

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	0.49537 (4)	0.26462 (3)	0.260441 (19)	0.04188 (18)	
B1	0.2081 (7)	0.8226 (4)	0.0862 (3)	0.0713 (13)	
B2	0.2989 (5)	0.2751 (4)	0.5691 (2)	0.0572 (10)	
C1	0.5758 (5)	0.1204 (3)	0.37557 (18)	0.0532 (8)	
C2	0.6673 (6)	0.0615 (4)	0.4203 (2)	0.0726 (12)	
H2	0.6203	−0.0149	0.4328	0.087*	
C3	0.8288 (7)	0.1186 (5)	0.4456 (2)	0.0807 (13)	
H3	0.8921	0.0805	0.4754	0.097*	
C4	0.8971 (6)	0.2322 (5)	0.4268 (2)	0.0715 (11)	
H4	1.0058	0.2719	0.4436	0.086*	
C5	0.7991 (5)	0.2847 (4)	0.3825 (2)	0.0637 (9)	
H5	0.8433	0.3618	0.3701	0.076*	
C6	0.4003 (5)	0.0685 (3)	0.34619 (18)	0.0543 (8)	
C7	0.2992 (7)	−0.0319 (4)	0.3697 (2)	0.0774 (12)	
H7	0.3426	−0.0721	0.4044	0.093*	
C8	0.1369 (7)	−0.0708 (5)	0.3416 (3)	0.0882 (15)	
H8	0.0683	−0.1367	0.3576	0.106*	
C9	0.0756 (6)	−0.0124 (4)	0.2897 (3)	0.0788 (13)	
H9	−0.0350	−0.0381	0.2701	0.095*	
C10	0.1788 (5)	0.0845 (4)	0.2669 (2)	0.0642 (9)	
H10	0.1369	0.1236	0.2313	0.077*	
C11	0.2700 (4)	0.4602 (3)	0.26873 (18)	0.0466 (7)	
C12	0.1730 (5)	0.5511 (4)	0.3006 (2)	0.0668 (10)	
H12	0.1169	0.5945	0.2713	0.080*	
C13	0.1602 (6)	0.5772 (4)	0.3762 (2)	0.0747 (12)	
H13	0.0949	0.6379	0.3984	0.090*	
C14	0.2444 (5)	0.5126 (4)	0.4179 (2)	0.0650 (10)	
H14	0.2368	0.5287	0.4689	0.078*	
C15	0.3399 (4)	0.4240 (3)	0.38420 (18)	0.0519 (8)	
H15	0.3972	0.3808	0.4131	0.062*	
C16	0.2887 (4)	0.4245 (3)	0.18751 (18)	0.0464 (7)	

C17	0.2861 (5)	0.5112 (4)	0.1416 (2)	0.0602 (9)	
H17	0.2694	0.5942	0.1602	0.072*	
C18	0.3090 (6)	0.4708 (4)	0.0674 (2)	0.0727 (11)	
H18	0.3097	0.5273	0.0352	0.087*	
C19	0.3305 (5)	0.3482 (4)	0.0413 (2)	0.0692 (11)	
H19	0.3437	0.3193	−0.0088	0.083*	
C20	0.3323 (5)	0.2684 (4)	0.0904 (2)	0.0611 (9)	
H20	0.3480	0.1848	0.0725	0.073*	
C21	0.7564 (4)	0.3415 (4)	0.16426 (18)	0.0511 (8)	
C22	0.8481 (5)	0.4169 (5)	0.1212 (2)	0.0709 (11)	
H22	0.9015	0.3802	0.0795	0.085*	
C23	0.8595 (6)	0.5468 (5)	0.1406 (3)	0.0787 (13)	
H23	0.9201	0.5987	0.1120	0.094*	
C24	0.7813 (6)	0.5986 (4)	0.2022 (3)	0.0747 (12)	
H24	0.7909	0.6862	0.2167	0.090*	
C25	0.6873 (5)	0.5201 (3)	0.2430 (2)	0.0582 (9)	
H25	0.6340	0.5560	0.2849	0.070*	
C26	0.7395 (4)	0.2022 (4)	0.14967 (17)	0.0507 (8)	
C27	0.8424 (5)	0.1326 (5)	0.1022 (2)	0.0754 (12)	
H27	0.9284	0.1734	0.0773	0.090*	
C28	0.8152 (7)	0.0010 (5)	0.0924 (3)	0.0868 (14)	
H28	0.8822	−0.0473	0.0606	0.104*	
C29	0.6890 (6)	−0.0562 (4)	0.1299 (2)	0.0748 (12)	
H29	0.6687	−0.1441	0.1241	0.090*	
C30	0.5918 (5)	0.0179 (3)	0.1767 (2)	0.0598 (9)	
H30	0.5053	−0.0220	0.2017	0.072*	
F1	0.2206 (7)	0.8026 (3)	0.15562 (17)	0.1338 (15)	
F2	0.0550 (4)	0.7601 (3)	0.05207 (18)	0.1028 (10)	
F3	0.3345 (5)	0.7722 (4)	0.0444 (2)	0.1279 (13)	
F4	0.2193 (4)	0.9489 (2)	0.08575 (18)	0.0921 (8)	
F5	0.4322 (11)	0.2699 (7)	0.6125 (7)	0.113 (4)	0.60 (2)
F6	0.312 (2)	0.2132 (10)	0.5016 (4)	0.141 (6)	0.60 (2)
F8	0.2847 (5)	0.3995 (3)	0.5705 (2)	0.1150 (11)	
F7	0.1557 (11)	0.2347 (11)	0.5970 (10)	0.160 (7)	0.60 (2)
N1	0.6436 (4)	0.2301 (3)	0.35638 (15)	0.0523 (7)	
N2	0.3391 (4)	0.1247 (3)	0.29465 (16)	0.0521 (7)	
N3	0.3538 (3)	0.3971 (2)	0.31056 (14)	0.0451 (6)	
N4	0.3126 (4)	0.3045 (3)	0.16283 (15)	0.0516 (7)	
N5	0.6716 (3)	0.3931 (3)	0.22333 (14)	0.0468 (6)	
N6	0.6162 (3)	0.1444 (3)	0.18753 (14)	0.0467 (6)	
F5'	0.4303 (17)	0.2429 (13)	0.5288 (12)	0.134 (7)	0.40 (2)
F6'	0.167 (2)	0.1857 (13)	0.5369 (11)	0.138 (8)	0.40 (2)
F7'	0.316 (3)	0.2394 (10)	0.6360 (4)	0.128 (9)	0.40 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0510 (3)	0.0333 (2)	0.0445 (3)	0.00823 (16)	0.01055 (16)	0.01354 (16)

B1	0.096 (3)	0.044 (2)	0.073 (3)	0.012 (2)	−0.005 (3)	0.008 (2)
B2	0.055 (2)	0.056 (2)	0.063 (3)	0.0074 (18)	−0.0015 (19)	0.0168 (19)
C1	0.081 (2)	0.0435 (17)	0.0424 (17)	0.0206 (16)	0.0174 (16)	0.0167 (14)
C2	0.103 (3)	0.064 (2)	0.067 (2)	0.034 (2)	0.019 (2)	0.036 (2)
C3	0.100 (3)	0.093 (3)	0.066 (3)	0.046 (3)	0.006 (2)	0.032 (2)
C4	0.072 (2)	0.088 (3)	0.061 (2)	0.024 (2)	−0.0003 (19)	0.023 (2)
C5	0.071 (2)	0.063 (2)	0.059 (2)	0.0103 (19)	0.0011 (18)	0.0181 (18)
C6	0.083 (2)	0.0375 (16)	0.0451 (17)	0.0098 (16)	0.0228 (16)	0.0129 (13)
C7	0.115 (4)	0.055 (2)	0.068 (3)	0.003 (2)	0.023 (2)	0.0326 (19)
C8	0.109 (4)	0.064 (3)	0.087 (3)	−0.017 (3)	0.027 (3)	0.022 (2)
C9	0.078 (3)	0.065 (3)	0.083 (3)	−0.014 (2)	0.015 (2)	0.003 (2)
C10	0.069 (2)	0.053 (2)	0.068 (2)	0.0019 (18)	0.0092 (19)	0.0074 (17)
C11	0.0481 (16)	0.0438 (17)	0.0495 (17)	0.0097 (13)	0.0006 (13)	0.0106 (14)
C12	0.074 (2)	0.062 (2)	0.069 (2)	0.0321 (19)	−0.0023 (19)	0.0069 (19)
C13	0.083 (3)	0.071 (3)	0.071 (3)	0.036 (2)	0.010 (2)	−0.002 (2)
C14	0.080 (2)	0.061 (2)	0.053 (2)	0.017 (2)	0.0138 (18)	0.0059 (17)
C15	0.0611 (19)	0.0512 (19)	0.0445 (17)	0.0114 (15)	0.0068 (15)	0.0091 (14)
C16	0.0474 (16)	0.0443 (17)	0.0488 (17)	0.0084 (13)	−0.0015 (13)	0.0112 (13)
C17	0.073 (2)	0.051 (2)	0.062 (2)	0.0183 (17)	−0.0029 (18)	0.0205 (16)
C18	0.093 (3)	0.077 (3)	0.058 (2)	0.019 (2)	−0.001 (2)	0.033 (2)
C19	0.081 (3)	0.080 (3)	0.047 (2)	0.013 (2)	−0.0019 (18)	0.0147 (19)
C20	0.080 (2)	0.052 (2)	0.0491 (19)	0.0117 (18)	−0.0048 (17)	0.0046 (16)
C21	0.0464 (16)	0.066 (2)	0.0421 (16)	0.0014 (15)	−0.0028 (13)	0.0187 (15)
C22	0.063 (2)	0.090 (3)	0.061 (2)	−0.013 (2)	0.0065 (18)	0.032 (2)
C23	0.075 (3)	0.087 (3)	0.078 (3)	−0.020 (2)	−0.004 (2)	0.049 (3)
C24	0.074 (3)	0.056 (2)	0.096 (3)	−0.0113 (19)	−0.018 (2)	0.033 (2)
C25	0.060 (2)	0.0474 (19)	0.067 (2)	−0.0014 (15)	−0.0043 (17)	0.0173 (16)
C26	0.0502 (17)	0.065 (2)	0.0389 (16)	0.0119 (15)	0.0017 (13)	0.0117 (14)
C27	0.064 (2)	0.103 (4)	0.060 (2)	0.021 (2)	0.0202 (19)	0.014 (2)
C28	0.094 (3)	0.092 (4)	0.075 (3)	0.043 (3)	0.017 (2)	−0.004 (3)
C29	0.101 (3)	0.059 (2)	0.066 (2)	0.032 (2)	0.006 (2)	0.0024 (19)
C30	0.078 (2)	0.0463 (19)	0.057 (2)	0.0190 (17)	0.0064 (18)	0.0067 (16)
F1	0.258 (5)	0.0714 (19)	0.0760 (19)	0.036 (2)	−0.022 (2)	0.0164 (15)
F2	0.103 (2)	0.094 (2)	0.105 (2)	−0.0224 (17)	0.0018 (17)	0.0294 (17)
F3	0.118 (3)	0.106 (3)	0.162 (3)	0.048 (2)	0.024 (2)	0.006 (2)
F4	0.110 (2)	0.0504 (13)	0.119 (2)	0.0081 (13)	0.0053 (17)	0.0272 (14)
F5	0.099 (5)	0.083 (4)	0.160 (9)	0.015 (3)	−0.059 (5)	0.029 (4)
F6	0.228 (17)	0.131 (8)	0.069 (4)	0.072 (10)	0.017 (6)	−0.005 (4)
F8	0.160 (3)	0.0683 (18)	0.127 (3)	0.0292 (19)	−0.006 (2)	0.0337 (17)
F7	0.088 (5)	0.144 (8)	0.277 (18)	0.016 (5)	0.080 (9)	0.114 (9)
N1	0.0717 (18)	0.0419 (14)	0.0486 (15)	0.0124 (13)	0.0089 (13)	0.0185 (12)
N2	0.0644 (17)	0.0405 (14)	0.0538 (16)	0.0104 (13)	0.0135 (13)	0.0125 (12)
N3	0.0511 (14)	0.0392 (13)	0.0465 (14)	0.0067 (11)	0.0038 (11)	0.0120 (11)
N4	0.0642 (17)	0.0432 (15)	0.0487 (15)	0.0112 (13)	−0.0019 (13)	0.0096 (12)
N5	0.0517 (14)	0.0453 (15)	0.0451 (14)	0.0034 (12)	−0.0015 (11)	0.0156 (11)
N6	0.0523 (14)	0.0466 (15)	0.0426 (14)	0.0109 (12)	0.0047 (11)	0.0096 (11)
F5'	0.090 (7)	0.138 (9)	0.160 (17)	0.014 (6)	0.058 (9)	−0.001 (8)
F6'	0.132 (12)	0.125 (10)	0.152 (14)	−0.037 (8)	−0.069 (11)	0.054 (10)
F7'	0.26 (3)	0.068 (6)	0.056 (4)	0.037 (9)	−0.016 (7)	0.010 (4)

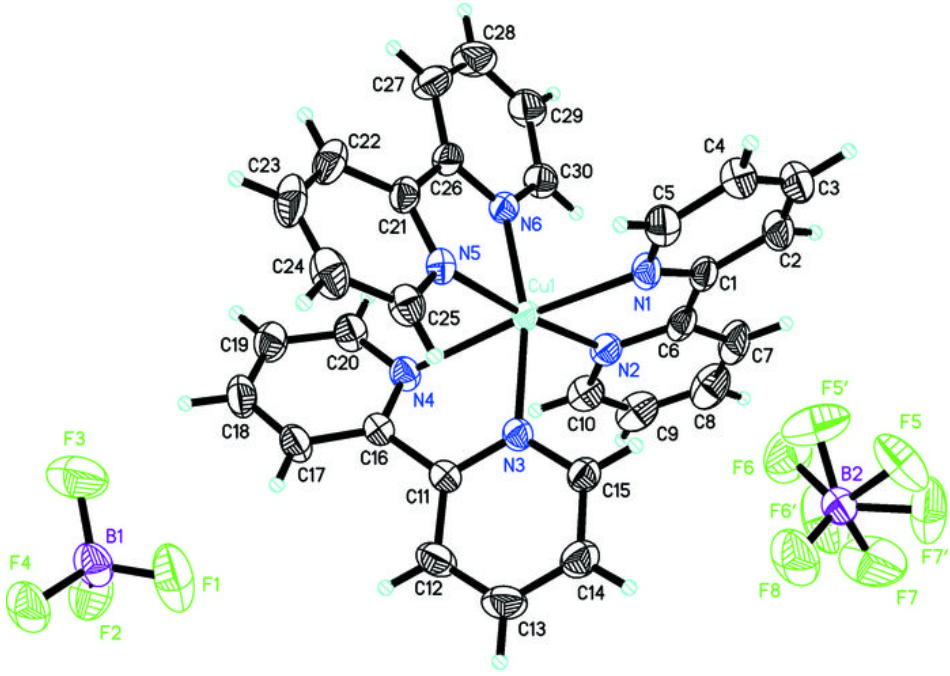
Geometric parameters (Å, °)

Cu1—N2	2.019 (3)	C11—C16	1.491 (4)
Cu1—N6	2.032 (3)	C12—C13	1.379 (6)
Cu1—N3	2.034 (3)	C12—H12	0.9300
Cu1—N5	2.044 (3)	C13—C14	1.364 (6)
Cu1—N1	2.239 (3)	C13—H13	0.9300
Cu1—N4	2.445 (3)	C14—C15	1.365 (5)
B1—F1	1.346 (6)	C14—H14	0.9300
B1—F4	1.362 (5)	C15—N3	1.345 (4)
B1—F3	1.378 (6)	C15—H15	0.9300
B1—F2	1.388 (6)	C16—N4	1.336 (4)
B2—F7	1.301 (7)	C16—C17	1.382 (5)
B2—F6	1.312 (8)	C17—C18	1.381 (6)
B2—F5'	1.330 (10)	C17—H17	0.9300
B2—F5	1.336 (7)	C18—C19	1.361 (6)
B2—F8	1.366 (5)	C18—H18	0.9300
B2—F6'	1.370 (11)	C19—C20	1.369 (6)
B2—F7'	1.376 (9)	C19—H19	0.9300
C1—N1	1.346 (4)	C20—N4	1.338 (5)
C1—C2	1.392 (5)	C20—H20	0.9300
C1—C6	1.482 (5)	C21—N5	1.355 (4)
C2—C3	1.377 (7)	C21—C22	1.383 (5)
C2—H2	0.9300	C21—C26	1.471 (5)
C3—C4	1.381 (7)	C22—C23	1.378 (7)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.375 (6)	C23—C24	1.362 (7)
C4—H4	0.9300	C23—H23	0.9300
C5—N1	1.334 (5)	C24—C25	1.385 (6)
C5—H5	0.9300	C24—H24	0.9300
C6—N2	1.346 (5)	C25—N5	1.345 (4)
C6—C7	1.397 (5)	C25—H25	0.9300
C7—C8	1.362 (7)	C26—N6	1.354 (4)
C7—H7	0.9300	C26—C27	1.390 (5)
C8—C9	1.366 (7)	C27—C28	1.390 (7)
C8—H8	0.9300	C27—H27	0.9300
C9—C10	1.371 (6)	C28—C29	1.363 (7)
C9—H9	0.9300	C28—H28	0.9300
C10—N2	1.347 (5)	C29—C30	1.379 (6)
C10—H10	0.9300	C29—H29	0.9300
C11—N3	1.351 (4)	C30—N6	1.335 (5)
C11—C12	1.381 (5)	C30—H30	0.9300
N2—Cu1—N6	94.42 (11)	C13—C12—C11	119.5 (4)
N2—Cu1—N3	91.40 (11)	C13—C12—H12	120.3
N6—Cu1—N3	165.91 (11)	C11—C12—H12	120.3
N2—Cu1—N5	173.96 (11)	C14—C13—C12	119.1 (4)
N6—Cu1—N5	80.24 (11)	C14—C13—H13	120.4
N3—Cu1—N5	94.44 (11)	C12—C13—H13	120.4

N2—Cu1—N1	77.41 (12)	C13—C14—C15	119.5 (4)
N6—Cu1—N1	92.18 (11)	C13—C14—H14	120.3
N3—Cu1—N1	101.62 (11)	C15—C14—H14	120.3
N5—Cu1—N1	99.84 (11)	N3—C15—C14	122.3 (3)
N2—Cu1—N4	99.54 (12)	N3—C15—H15	118.9
N6—Cu1—N4	92.01 (10)	C14—C15—H15	118.9
N3—Cu1—N4	74.35 (10)	N4—C16—C17	122.7 (3)
N5—Cu1—N4	83.56 (10)	N4—C16—C11	115.4 (3)
N1—Cu1—N4	175.00 (10)	C17—C16—C11	121.9 (3)
F1—B1—F4	110.8 (4)	C18—C17—C16	118.0 (4)
F1—B1—F3	110.2 (5)	C18—C17—H17	121.0
F4—B1—F3	109.9 (5)	C16—C17—H17	121.0
F1—B1—F2	110.8 (5)	C19—C18—C17	119.9 (4)
F4—B1—F2	109.4 (4)	C19—C18—H18	120.1
F3—B1—F2	105.6 (4)	C17—C18—H18	120.1
F7—B2—F6	111.1 (8)	C18—C19—C20	118.5 (4)
F7—B2—F5'	146.0 (9)	C18—C19—H19	120.8
F6—B2—F5'	46.2 (6)	C20—C19—H19	120.8
F7—B2—F5	111.1 (7)	N4—C20—C19	123.3 (4)
F6—B2—F5	112.0 (7)	N4—C20—H20	118.3
F5'—B2—F5	69.5 (8)	C19—C20—H20	118.3
F7—B2—F8	102.1 (5)	N5—C21—C22	121.1 (4)
F6—B2—F8	111.6 (5)	N5—C21—C26	115.0 (3)
F5'—B2—F8	109.9 (7)	C22—C21—C26	123.9 (4)
F5—B2—F8	108.5 (5)	C23—C22—C21	119.3 (4)
F7—B2—F6'	50.8 (7)	C23—C22—H22	120.3
F6—B2—F6'	60.3 (8)	C21—C22—H22	120.3
F5'—B2—F6'	102.3 (10)	C24—C23—C22	119.4 (4)
F5—B2—F6'	132.7 (8)	C24—C23—H23	120.3
F8—B2—F6'	117.7 (8)	C22—C23—H23	120.3
F7—B2—F7'	65.3 (9)	C23—C24—C25	119.7 (4)
F6—B2—F7'	130.9 (6)	C23—C24—H24	120.2
F5'—B2—F7'	107.9 (10)	C25—C24—H24	120.2
F5—B2—F7'	45.8 (7)	N5—C25—C24	121.4 (4)
F8—B2—F7'	117.0 (5)	N5—C25—H25	119.3
F6'—B2—F7'	100.7 (9)	C24—C25—H25	119.3
N1—C1—C2	121.1 (4)	N6—C26—C27	121.2 (4)
N1—C1—C6	115.7 (3)	N6—C26—C21	114.9 (3)
C2—C1—C6	123.3 (3)	C27—C26—C21	123.9 (4)
C3—C2—C1	118.7 (4)	C28—C27—C26	119.1 (4)
C3—C2—H2	120.7	C28—C27—H27	120.4
C1—C2—H2	120.7	C26—C27—H27	120.4
C2—C3—C4	120.1 (4)	C29—C28—C27	119.1 (4)
C2—C3—H3	119.9	C29—C28—H28	120.4
C4—C3—H3	119.9	C27—C28—H28	120.4
C5—C4—C3	117.9 (4)	C28—C29—C30	119.1 (4)
C5—C4—H4	121.1	C28—C29—H29	120.4
C3—C4—H4	121.1	C30—C29—H29	120.4
N1—C5—C4	123.0 (4)	N6—C30—C29	122.9 (4)

N1—C5—H5	118.5	N6—C30—H30	118.5
C4—C5—H5	118.5	C29—C30—H30	118.5
N2—C6—C7	120.1 (4)	C5—N1—C1	119.2 (3)
N2—C6—C1	116.2 (3)	C5—N1—Cu1	128.7 (2)
C7—C6—C1	123.6 (4)	C1—N1—Cu1	110.2 (2)
C8—C7—C6	119.8 (4)	C6—N2—C10	119.4 (3)
C8—C7—H7	120.1	C6—N2—Cu1	118.0 (2)
C6—C7—H7	120.1	C10—N2—Cu1	122.6 (3)
C7—C8—C9	119.5 (4)	C15—N3—C11	118.6 (3)
C7—C8—H8	120.2	C15—N3—Cu1	122.2 (2)
C9—C8—H8	120.2	C11—N3—Cu1	119.2 (2)
C8—C9—C10	119.3 (4)	C16—N4—C20	117.6 (3)
C8—C9—H9	120.3	C16—N4—Cu1	102.3 (2)
C10—C9—H9	120.3	C20—N4—Cu1	125.5 (2)
N2—C10—C9	121.8 (4)	C25—N5—C21	118.9 (3)
N2—C10—H10	119.1	C25—N5—Cu1	126.4 (2)
C9—C10—H10	119.1	C21—N5—Cu1	113.6 (2)
N3—C11—C12	121.0 (3)	C30—N6—C26	118.5 (3)
N3—C11—C16	115.9 (3)	C30—N6—Cu1	126.8 (2)
C12—C11—C16	123.1 (3)	C26—N6—Cu1	114.6 (2)

Fig. 1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