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Acetonitrilebis(2,9-dimethylphenanthroline)copper(II) bis(tetrafluoridoborate) acetonitrile disolvate

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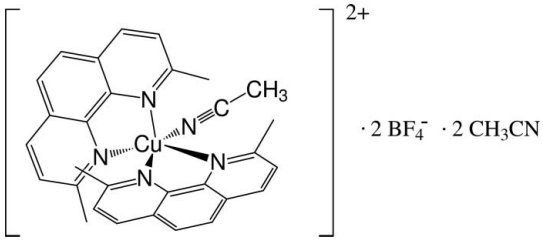
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.040; wR factor = 0.098; data-to-parameter ratio = 16.6.

In the title compound, $[Cu(CH_3CN)(C_{14}H_{12}N_2)_2](BF_4)_2\cdot 2CH_3CN$, the Cu^{II} atom shows a distorted CuN_5 square-pyramidal geometry with the acetonitrile N atom in an equatorial site, which differs substantially from the distorted trigonal-bipyramidal arrangement usually observed for five-coordinate complexes of Cu^{II} with two phenanthroline-type ligands and one other ligand. The B atom of one of the BF_4^- anions is disordered over two sites in a 0.825 (2):0.175 (2) ratio. In the crystal, C—H···F hydrogen bonds help to establish the packing.

Related literature

For related structures, see: Bush *et al.* (2001); Vega *et al.* (1985); Aligo *et al.* (2005). For background, see: Kepert (1973); Rossi & Hoffman (1975); James & Williams (1961).



Experimental

Crystal data

$[Cu(C_2H_3N)(C_{14}H_{12}N_2)_2](BF_4)_2\cdot 2C_2H_3N$
M_r = 776.83
Triclinic, $P\overline{1}$
a = 11.2865 (19) Å
b = 12.070 (2) Å
c = 13.802 (2) Å
α = 72.843 (15)°
β = 83.746 (15)°
γ = 73.933 (15)°
V = 1725.7 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Sapphire diffractometer
Absorption correction: multi-scan (*SCALE3 ABSPACK* in *CrysAlis RED*; Oxford Diffraction, 2006).
T_{min} = 0.997, T_{max} = 1.000 (expected range = 0.864–0.867)
10543 measured reflections
8129 independent reflections
4935 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.098
S = 0.89
8129 reflections
489 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N5	2.0123 (18)	N3—C25	1.351 (3)
Cu1—N2	2.0297 (17)	N3—C28	1.359 (3)
Cu1—N3	2.0305 (18)	N4—C16	1.333 (2)
Cu1—N4	2.0348 (17)	N4—C27	1.365 (3)
Cu1—N1	2.1760 (18)		
N5—Cu1—N2	84.42 (7)	N3—Cu1—N4	81.25 (7)
N5—Cu1—N3	89.07 (7)	N5—Cu1—N1	100.93 (7)
N2—Cu1—N3	165.23 (7)	N2—Cu1—N1	80.17 (7)
N5—Cu1—N4	150.90 (7)	N3—Cu1—N1	114.15 (7)
N2—Cu1—N4	98.14 (7)	N4—Cu1—N1	108.09 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12C···F8^{i}	0.96	2.36	3.120 (3)	135
C18—H18···F5^{ii}	0.93	2.36	3.279 (3)	171
C20—H20···F8^{ii}	0.93	2.53	3.423 (3)	161
C30—H30A···F8	0.96	2.47	3.375 (4)	158
C30—H30B···F6^{iii}	0.96	2.38	3.314 (3)	165
C32—H32B···F7^{iv}	0.96	2.37	3.191 (3)	143

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

I thank Dr Guy Crundwell for his assistance with the disorder modeling, and with preparation of this manuscript, and I thank Dr Laura Pence for helpful discussions concerning the geometry of the complex.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2926).

References

Aligo, J. A., Smith, L., Eglin, J. E. & Pence, L. E. (2005). *Inorg. Chem.* **44**, 4001–4007.
Bush, P. M., Whitehead, J. P., Pink, C. C., Gramm, E. C., Eglin, J. C., Watton, S. P. & Pence, L. E. (2001). *Inorg. Chem.* **40**, 1871–1877.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
James, B. R. & Williams, R. J. P. (1961). *J. Chem. Soc.* pp. 2007–2019.
Kepert, D. L. (1973). *Inorg. Chem.* **12**, 1938–1942.
Oxford Diffraction (2006). *CrysAlis CCD, CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Rossi, A. R. & Hoffman, R. (1975). *Inorg. Chem.* **14**, 365–374.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vega, I. E. D., Gale, P. A., Lighta, M. E. & Loeb, S. J. (1985). *Chem. Commun.* **39**, 4913–4915.

supporting information

Acta Cryst. (2009). E**65**, m585–m586 [doi:10.1107/S1600536809012331]

Acetonitrilebis(2,9-dimethylphenanthroline)copper(II) bis(tetrafluoridoborate) acetonitrile disolvate

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S1. Comment

The copper-containing cation (Fig. 1) of the title compound, (I), consists of a 5-coordinate Cu center, with the geometry about copper being best described (Kepert, 1973) as distorted square pyramidal, rather than as a distorted TBP structure, which is most commonly observed for five-coordinate copper bis-phenanthroline complexes (Bush, *et al.*, 2001). Most of the distortion from idealized square pyramidal can be explained in terms of the restricted bite angles of the rigid phenanthroline rings. It is assumed that steric strain associated with the presence of the 2,9-dimethyl groups on the ligand overrides electronic considerations (Rossi and Hoffman, 1975), resulting in formation of the disfavored square pyramidal geometry for the d^9 complex. The steric strain inherent in the structure is also reflected in the copper being located considerably outside of the normal coordination plane of the phenanthroline [0.470 (1) and 0.636 (1)Å from the least squares planes of the two rings], and in a clear bowing of the phenanthroline ligand itself.

The observation of an electronically high-energy structure is fully consistent with electrochemical data (James and Williams, 1961) which show the 2,9-disubstituted phenanthroline complex to be significantly easier to reduce than the analogous complexes lacking the 2,9- substituents. Reduction of the $[Cu(neocuproine)_2(solv)]^{2+}$ complexes affords the air-stable $[Cu(neocuproine)_2]^{+}$ species, which adopt pseudo-tetrahedral geometries that alleviate the steric strain between the substituents.

In the structure of (I), close contact of the disordered BF_4^- and the coordinated CH_3CN suggest that a C—H hydrogen bonding interaction exists (see, for example: Vega, *et al.*, 1985). Similar interactions between BF_4^- ions and Cu-bound acetonitrile ligands have been observed previously (Aligo, *et al.*, 2005). The packing of (I) is shown in Fig. 2 and the H bonds are listed in Table 2.

S2. Experimental

Copper (II) tetrafluoroborate hydrate (0.100 g, 0.42 mmol) was dissolved in 5 ml of acetonitrile and 2,9-dimethyl-phenanthroline (0.190 g, 0.92 mmol) was added as a solution in 5 ml of acetonitrile. Vapor diffusion of ether into the solution afforded green blocks of (I). Yield 0.182 g (56%).

S3. Refinement

All H atoms were included at calculated positions and were allowed to ride with their C atoms during refinement. The structure exhibits disorder of one of the two BF_4^- counterions. The disorder was modeled using two identical constrained fragments which shared a common F atom. Occupancy refinement indicated a relative population of 0.175 (2) to 0.825 (2) for the two positions.

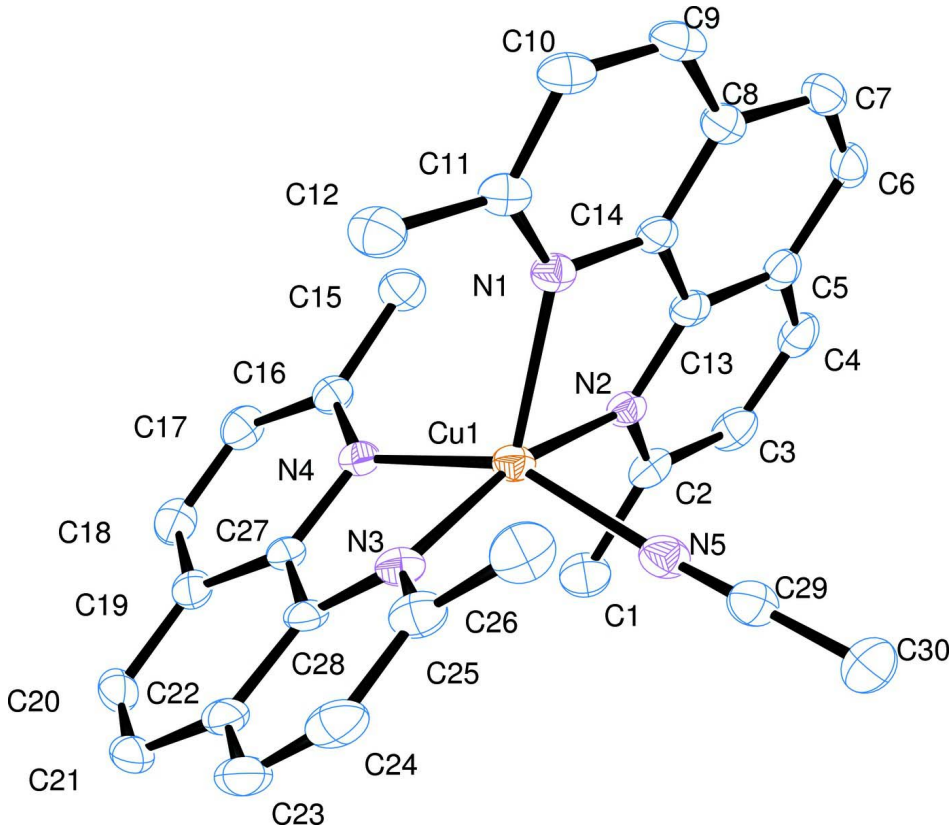

Figure 1

View of the cation in (I) with H atoms omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

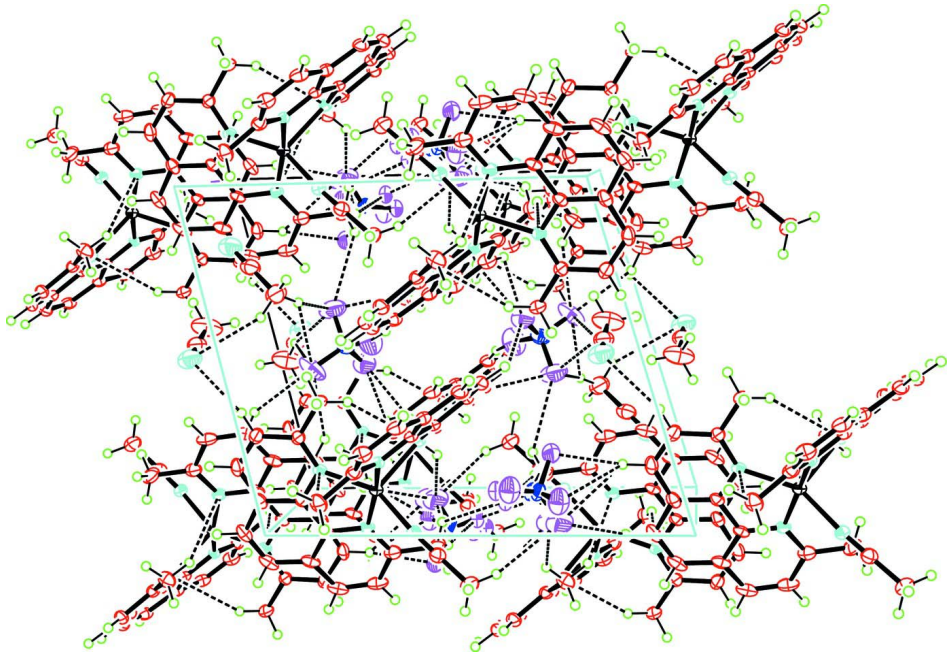

Figure 2

The packing for (I): H atoms are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

Acetonitrilebis(2,9-dimethylphenanthroline)copper(II) bis(tetrafluoroborate) acetonitrile disolvate

Crystal data

$[Cu(C_2H_3N)(C_{14}H_{12}N_2)_2](BF_4)_2\cdot 2C_2H_3N$
$M_r = 776.83$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 11.2865\ (19)$ Å
$b = 12.070\ (2)$ Å
$c = 13.802\ (2)$ Å
$\alpha = 72.843\ (15)°$
$\beta = 83.746\ (15)°$
$\gamma = 73.933\ (15)°$
$V = 1725.7\ (5)$ Å^3
$Z = 2$
$F(000) = 794$
$D_x = 1.495$ Mg m^{-3}
Melting point > 523 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4074 reflections
$\theta = 3.9–32.1°$
$\mu = 0.71$ mm^{-1}
$T = 293$ K
Block, green
0.3 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Sapphire diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SCALE3 ABSPACK in *CrysAlis RED*; Oxford Diffraction, 2006).
$T_{min} = 0.997$, $T_{max} = 1.000$
10543 measured reflections
8129 independent reflections
4935 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 32.2°$, $\theta_{min} = 3.9°$
$h = -16\rightarrow13$
$k = -17\rightarrow17$
$l = -20\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.098$
$S = 0.89$
8129 reflections
489 parameters
30 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

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

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.22719 (2)	0.09638 (2)	0.73647 (2)	0.02082 (9)	
N1	0.27230 (16)	0.23116 (14)	0.60440 (13)	0.0205 (4)	

N2	0.05462 (16)	0.19388 (14)	0.69210 (13)	0.0193 (4)
C1	−0.0467 (2)	0.0955 (2)	0.84546 (18)	0.0323 (6)
H1A	−0.0745	0.0276	0.8442	0.048*
H1B	−0.0993	0.1359	0.8909	0.048*
H1C	0.0365	0.0687	0.8683	0.048*
C2	−0.0512 (2)	0.17993 (18)	0.74111 (18)	0.0257 (5)
C3	−0.1658 (2)	0.24420 (19)	0.69496 (19)	0.0289 (5)
H3	−0.2392	0.2375	0.7311	0.035*
C4	−0.1685 (2)	0.31611 (18)	0.59724 (18)	0.0284 (5)
H4	−0.2437	0.3563	0.5665	0.034*
C5	−0.0576 (2)	0.32924 (17)	0.54323 (17)	0.0230 (5)
C6	−0.0512 (2)	0.40115 (17)	0.44062 (17)	0.0275 (5)
H6	−0.1233	0.4388	0.4046	0.033*
C7	0.0580 (2)	0.41503 (18)	0.39547 (18)	0.0273 (5)
H7	0.0600	0.4603	0.3282	0.033*
C8	0.1698 (2)	0.36192 (17)	0.44850 (16)	0.0227 (5)
C9	0.2844 (2)	0.38422 (17)	0.40945 (17)	0.0273 (5)
H9	0.2910	0.4319	0.3435	0.033*
C10	0.3853 (2)	0.33573 (18)	0.46848 (17)	0.0268 (5)
H10	0.4598	0.3539	0.4439	0.032*
C11	0.3777 (2)	0.25780 (17)	0.56708 (17)	0.0227 (5)
C12	0.4879 (2)	0.2062 (2)	0.63242 (19)	0.0320 (6)
H12A	0.4655	0.1590	0.6974	0.048*
H12B	0.5170	0.2701	0.6412	0.048*
H12C	0.5518	0.1564	0.6007	0.048*
C13	0.05311 (19)	0.26752 (16)	0.59555 (16)	0.0203 (5)
C14	0.16866 (19)	0.28576 (16)	0.54751 (16)	0.0197 (5)
N3	0.37614 (16)	−0.03179 (14)	0.80310 (14)	0.0224 (4)
N4	0.23061 (15)	0.15164 (14)	0.86165 (13)	0.0193 (4)
C15	0.1143 (2)	0.36074 (17)	0.80198 (17)	0.0273 (5)
H15A	0.1568	0.3556	0.7387	0.041*
H15B	0.1200	0.4320	0.8166	0.041*
H15C	0.0292	0.3637	0.7975	0.041*
C16	0.17194 (19)	0.25310 (17)	0.88480 (16)	0.0209 (5)
C17	0.1641 (2)	0.25959 (19)	0.98550 (17)	0.0263 (5)
H17	0.1211	0.3307	1.0002	0.032*
C18	0.2184 (2)	0.1634 (2)	1.06205 (18)	0.0280 (5)
H18	0.2099	0.1675	1.1288	0.034*
C19	0.2881 (2)	0.05700 (18)	1.03802 (17)	0.0237 (5)
C20	0.3561 (2)	−0.04595 (19)	1.11054 (18)	0.0287 (5)
H20	0.3505	−0.0479	1.1787	0.034*
C21	0.4291 (2)	−0.14124 (19)	1.08054 (18)	0.0309 (6)
H21	0.4723	−0.2079	1.1287	0.037*
C22	0.4403 (2)	−0.14037 (18)	0.97633 (18)	0.0266 (5)
C23	0.5219 (2)	−0.23138 (19)	0.9381 (2)	0.0327 (6)
H23	0.5680	−0.3003	0.9823	0.039*
C24	0.5322 (2)	−0.21712 (18)	0.8365 (2)	0.0329 (6)
H24	0.5889	−0.2751	0.8116	0.039*

C25	0.4591 (2)	−0.11654 (18)	0.76774 (18)	0.0284 (5)	
C26	0.4755 (2)	−0.1021 (2)	0.65667 (19)	0.0356 (6)	
H26A	0.4279	−0.0242	0.6207	0.053*	
H26B	0.4482	−0.1628	0.6403	0.053*	
H26C	0.5611	−0.1099	0.6373	0.053*	
C27	0.29190 (19)	0.05730 (17)	0.93622 (16)	0.0200 (5)	
C28	0.37000 (19)	−0.04304 (16)	0.90432 (17)	0.0211 (5)	
N5	0.19544 (17)	−0.02025 (15)	0.67040 (14)	0.0272 (4)	
C29	0.1858 (2)	−0.08244 (18)	0.62641 (18)	0.0280 (5)	
C30	0.1774 (2)	−0.1635 (2)	0.5691 (2)	0.0381 (6)	
H30A	0.2111	−0.1384	0.5018	0.057*	
H30B	0.0925	−0.1621	0.5656	0.057*	
H30C	0.2230	−0.2435	0.6022	0.057*	
N6	0.1570 (2)	0.8133 (2)	0.92492 (19)	0.0532 (6)	
C31	0.1324 (2)	0.7532 (2)	0.8848 (2)	0.0393 (6)	
C32	0.1015 (3)	0.6748 (2)	0.8345 (2)	0.0493 (7)	
H32A	0.1717	0.6443	0.7951	0.074*	
H32B	0.0336	0.7193	0.7907	0.074*	
H32C	0.0788	0.6091	0.8845	0.074*	
N7	0.1493 (2)	0.4854 (2)	0.0983 (2)	0.0571 (7)	
C33	0.2350 (3)	0.5198 (2)	0.0862 (2)	0.0405 (6)	
C34	0.3440 (3)	0.5640 (3)	0.0680 (3)	0.0680 (10)	
H34A	0.3701	0.5745	−0.0019	0.102*	
H34B	0.4085	0.5073	0.1103	0.102*	
H34C	0.3258	0.6395	0.0835	0.102*	
B1	0.5835 (3)	0.5036 (2)	0.2591 (2)	0.0350 (7)	
F1	0.66138 (15)	0.48303 (17)	0.33530 (13)	0.0687 (5)	
F2	0.46588 (13)	0.56703 (13)	0.28167 (12)	0.0502 (4)	
F3	0.57688 (17)	0.39330 (14)	0.25247 (15)	0.0712 (5)	
F4	0.62598 (14)	0.56564 (15)	0.16773 (13)	0.0653 (5)	
B2	0.1702 (4)	0.0967 (3)	0.3432 (3)	0.0336 (9)	0.825 (2)
F5	0.20526 (15)	0.19999 (12)	0.28948 (11)	0.0480 (4)	0.825 (2)
F6	0.1266 (2)	0.10525 (16)	0.43944 (14)	0.0446 (5)	0.825 (2)
F7	0.07552 (17)	0.08275 (18)	0.29426 (15)	0.0543 (6)	0.825 (2)
F8	0.2690 (2)	−0.00073 (18)	0.34420 (18)	0.0602 (6)	0.825 (2)
B2B	0.2011 (15)	0.0932 (13)	0.3623 (11)	0.0336 (9)	0.175 (2)
F5B	0.20526 (15)	0.19999 (12)	0.28948 (11)	0.0480 (4)	0.175 (2)
F6B	0.2824 (8)	0.0556 (7)	0.4379 (6)	0.0446 (5)	0.175 (2)
F7B	0.0796 (9)	0.1141 (10)	0.4016 (9)	0.0543 (6)	0.175 (2)
F8B	0.2038 (10)	0.0053 (9)	0.3170 (9)	0.0602 (6)	0.175 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02490 (16)	0.01560 (12)	0.02076 (17)	−0.00460 (10)	0.00029 (11)	−0.00420 (9)
N1	0.0239 (10)	0.0171 (8)	0.0204 (10)	−0.0049 (7)	0.0026 (8)	−0.0064 (7)
N2	0.0234 (10)	0.0165 (8)	0.0197 (10)	−0.0072 (7)	0.0024 (8)	−0.0068 (7)
C1	0.0300 (13)	0.0371 (13)	0.0304 (15)	−0.0168 (11)	0.0073 (12)	−0.0053 (10)

C2	0.0280 (13)	0.0222 (10)	0.0316 (14)	−0.0113 (9)	0.0017 (11)	−0.0109 (9)
C3	0.0214 (12)	0.0273 (11)	0.0413 (16)	−0.0100 (9)	0.0011 (11)	−0.0117 (10)
C4	0.0257 (13)	0.0201 (10)	0.0420 (16)	−0.0031 (9)	−0.0104 (11)	−0.0115 (10)
C5	0.0245 (12)	0.0193 (10)	0.0284 (14)	−0.0062 (9)	−0.0035 (10)	−0.0097 (8)
C6	0.0356 (14)	0.0180 (10)	0.0285 (14)	−0.0017 (9)	−0.0153 (11)	−0.0055 (9)
C7	0.0388 (15)	0.0200 (10)	0.0215 (13)	−0.0054 (10)	−0.0049 (11)	−0.0037 (8)
C8	0.0319 (13)	0.0158 (9)	0.0193 (12)	−0.0032 (9)	0.0008 (10)	−0.0067 (8)
C9	0.0395 (14)	0.0189 (10)	0.0197 (13)	−0.0063 (10)	0.0072 (11)	−0.0039 (8)
C10	0.0290 (13)	0.0224 (10)	0.0267 (14)	−0.0088 (9)	0.0092 (11)	−0.0051 (9)
C11	0.0238 (12)	0.0176 (10)	0.0244 (13)	−0.0026 (9)	0.0056 (10)	−0.0070 (8)
C12	0.0243 (13)	0.0325 (12)	0.0345 (15)	−0.0076 (10)	0.0019 (11)	−0.0030 (10)
C13	0.0252 (12)	0.0140 (9)	0.0229 (13)	−0.0050 (8)	0.0007 (10)	−0.0077 (8)
C14	0.0249 (12)	0.0128 (9)	0.0219 (13)	−0.0038 (8)	−0.0002 (10)	−0.0068 (8)
N3	0.0248 (10)	0.0158 (8)	0.0253 (12)	−0.0048 (7)	0.0023 (9)	−0.0052 (7)
N4	0.0187 (9)	0.0168 (8)	0.0216 (11)	−0.0059 (7)	0.0009 (8)	−0.0035 (7)
C15	0.0319 (13)	0.0185 (10)	0.0298 (14)	−0.0018 (9)	−0.0015 (11)	−0.0084 (9)
C16	0.0197 (11)	0.0217 (10)	0.0223 (13)	−0.0074 (8)	0.0030 (10)	−0.0070 (8)
C17	0.0279 (13)	0.0281 (11)	0.0268 (14)	−0.0101 (10)	0.0042 (11)	−0.0127 (9)
C18	0.0308 (13)	0.0395 (13)	0.0195 (14)	−0.0191 (11)	0.0062 (11)	−0.0099 (10)
C19	0.0239 (12)	0.0296 (11)	0.0195 (13)	−0.0161 (9)	0.0013 (10)	−0.0017 (9)
C20	0.0298 (13)	0.0368 (13)	0.0192 (14)	−0.0186 (10)	−0.0047 (11)	0.0036 (9)
C21	0.0290 (13)	0.0283 (12)	0.0311 (16)	−0.0162 (10)	−0.0108 (11)	0.0099 (9)
C22	0.0215 (12)	0.0192 (10)	0.0366 (15)	−0.0101 (9)	−0.0061 (11)	0.0022 (9)
C23	0.0290 (13)	0.0185 (10)	0.0454 (18)	−0.0078 (9)	−0.0078 (12)	0.0028 (10)
C24	0.0242 (13)	0.0177 (10)	0.0544 (19)	−0.0018 (9)	−0.0023 (12)	−0.0092 (10)
C25	0.0262 (13)	0.0215 (10)	0.0361 (16)	−0.0056 (9)	0.0032 (11)	−0.0079 (9)
C26	0.0347 (14)	0.0294 (12)	0.0431 (17)	−0.0020 (11)	0.0056 (13)	−0.0186 (11)
C27	0.0211 (11)	0.0188 (9)	0.0205 (13)	−0.0105 (8)	−0.0007 (10)	−0.0011 (8)
C28	0.0219 (11)	0.0164 (9)	0.0241 (14)	−0.0105 (8)	−0.0005 (10)	0.0010 (8)
N5	0.0371 (11)	0.0189 (9)	0.0232 (11)	−0.0034 (8)	0.0008 (9)	−0.0063 (7)
C29	0.0303 (13)	0.0233 (11)	0.0271 (15)	−0.0045 (9)	−0.0017 (11)	−0.0041 (9)
C30	0.0491 (16)	0.0300 (12)	0.0393 (17)	−0.0109 (11)	−0.0029 (13)	−0.0146 (11)
N6	0.0573 (16)	0.0383 (13)	0.0632 (18)	−0.0169 (12)	0.0008 (13)	−0.0097 (12)
C31	0.0380 (15)	0.0279 (12)	0.0457 (18)	−0.0086 (11)	0.0070 (13)	−0.0037 (11)
C32	0.0546 (19)	0.0414 (15)	0.055 (2)	−0.0162 (14)	0.0111 (16)	−0.0195 (13)
N7	0.0549 (16)	0.0420 (13)	0.078 (2)	−0.0183 (13)	0.0175 (14)	−0.0231 (13)
C33	0.0471 (17)	0.0280 (12)	0.0450 (18)	−0.0105 (12)	0.0058 (14)	−0.0099 (11)
C34	0.053 (2)	0.0423 (16)	0.101 (3)	−0.0180 (15)	−0.0185 (19)	0.0030 (17)
B1	0.0279 (16)	0.0293 (14)	0.043 (2)	−0.0088 (12)	0.0002 (14)	−0.0022 (12)
F1	0.0476 (10)	0.0914 (14)	0.0596 (12)	−0.0102 (10)	−0.0204 (9)	−0.0101 (10)
F2	0.0346 (9)	0.0468 (9)	0.0636 (12)	−0.0047 (7)	0.0037 (8)	−0.0139 (8)
F3	0.0778 (13)	0.0413 (9)	0.0996 (16)	−0.0214 (9)	0.0141 (11)	−0.0272 (9)
F4	0.0410 (10)	0.0648 (11)	0.0601 (12)	−0.0121 (8)	0.0031 (9)	0.0246 (9)
B2	0.042 (3)	0.0327 (15)	0.026 (2)	−0.0028 (16)	0.0009 (17)	−0.0152 (14)
F5	0.0704 (11)	0.0442 (9)	0.0360 (10)	−0.0262 (8)	0.0093 (8)	−0.0143 (7)
F6	0.0712 (14)	0.0388 (9)	0.0236 (11)	−0.0134 (9)	0.0036 (10)	−0.0110 (8)
F7	0.0470 (12)	0.0763 (14)	0.0504 (14)	−0.0257 (10)	−0.0004 (10)	−0.0249 (10)
F8	0.0393 (13)	0.0447 (10)	0.0828 (17)	0.0122 (11)	0.0014 (12)	−0.0196 (10)

B2B	0.042 (3)	0.0327 (15)	0.026 (2)	−0.0028 (16)	0.0009 (17)	−0.0152 (14)
F5B	0.0704 (11)	0.0442 (9)	0.0360 (10)	−0.0262 (8)	0.0093 (8)	−0.0143 (7)
F6B	0.0712 (14)	0.0388 (9)	0.0236 (11)	−0.0134 (9)	0.0036 (10)	−0.0110 (8)
F7B	0.0470 (12)	0.0763 (14)	0.0504 (14)	−0.0257 (10)	−0.0004 (10)	−0.0249 (10)
F8B	0.0393 (13)	0.0447 (10)	0.0828 (17)	0.0122 (11)	0.0014 (12)	−0.0196 (10)

Geometric parameters (Å, º)

Cu1—N5	2.0123 (18)	C18—C19	1.419 (3)
Cu1—N2	2.0297 (17)	C18—H18	0.9300
Cu1—N3	2.0305 (18)	C19—C27	1.400 (3)
Cu1—N4	2.0348 (17)	C19—C20	1.429 (3)
Cu1—N1	2.1760 (18)	C20—C21	1.362 (3)
N1—C11	1.328 (3)	C20—H20	0.9300
N1—C14	1.374 (3)	C21—C22	1.427 (3)
N2—C2	1.334 (3)	C21—H21	0.9300
N2—C13	1.365 (3)	C22—C28	1.402 (3)
C1—C2	1.496 (3)	C22—C23	1.417 (3)
C1—H1A	0.9600	C23—C24	1.357 (3)
C1—H1B	0.9600	C23—H23	0.9300
C1—H1C	0.9600	C24—C25	1.411 (3)
C2—C3	1.419 (3)	C24—H24	0.9300
C3—C4	1.370 (3)	C25—C26	1.488 (3)
C3—H3	0.9300	C26—H26A	0.9600
C4—C5	1.408 (3)	C26—H26B	0.9600
C4—H4	0.9300	C26—H26C	0.9600
C5—C13	1.415 (3)	C27—C28	1.441 (3)
C5—C6	1.432 (3)	N5—C29	1.128 (3)
C6—C7	1.350 (3)	C29—C30	1.455 (3)
C6—H6	0.9300	C30—H30A	0.9600
C7—C8	1.420 (3)	C30—H30B	0.9600
C7—H7	0.9300	C30—H30C	0.9600
C8—C14	1.405 (3)	N6—C31	1.137 (3)
C8—C9	1.411 (3)	C31—C32	1.458 (4)
C9—C10	1.362 (3)	C32—H32A	0.9600
C9—H9	0.9300	C32—H32B	0.9600
C10—C11	1.417 (3)	C32—H32C	0.9600
C10—H10	0.9300	N7—C33	1.132 (3)
C11—C12	1.494 (3)	C33—C34	1.441 (4)
C12—H12A	0.9600	C34—H34A	0.9600
C12—H12B	0.9600	C34—H34B	0.9600
C12—H12C	0.9600	C34—H34C	0.9600
C13—C14	1.440 (3)	B1—F1	1.367 (3)
N3—C25	1.351 (3)	B1—F4	1.375 (3)
N3—C28	1.359 (3)	B1—F3	1.383 (3)
N4—C16	1.333 (2)	B1—F2	1.390 (3)
N4—C27	1.365 (3)	B2—F8	1.376 (4)
C15—C16	1.495 (3)	B2—F6	1.388 (4)

C15—H15A	0.9600	B2—F5	1.387 (4)
C15—H15B	0.9600	B2—F7	1.397 (4)
C15—H15C	0.9600	B2B—F6B	1.355 (14)
C16—C17	1.407 (3)	B2B—F8B	1.372 (14)
C17—C18	1.365 (3)	B2B—F7B	1.402 (15)
C17—H17	0.9300		

N5—Cu1—N2	84.42 (7)	C17—C16—C15	120.15 (18)
N5—Cu1—N3	89.07 (7)	C18—C17—C16	121.2 (2)
N2—Cu1—N3	165.23 (7)	C18—C17—H17	119.4
N5—Cu1—N4	150.90 (7)	C16—C17—H17	119.4
N2—Cu1—N4	98.14 (7)	C17—C18—C19	118.8 (2)
N3—Cu1—N4	81.25 (7)	C17—C18—H18	120.6
N5—Cu1—N1	100.93 (7)	C19—C18—H18	120.6
N2—Cu1—N1	80.17 (7)	C27—C19—C18	116.6 (2)
N3—Cu1—N1	114.15 (7)	C27—C19—C20	119.6 (2)
N4—Cu1—N1	108.09 (6)	C18—C19—C20	123.7 (2)
C11—N1—C14	118.58 (18)	C21—C20—C19	120.5 (2)
C11—N1—Cu1	132.80 (14)	C21—C20—H20	119.8
C14—N1—Cu1	108.16 (13)	C19—C20—H20	119.8
C2—N2—C13	119.90 (19)	C20—C21—C22	121.0 (2)
C2—N2—Cu1	126.65 (15)	C20—C21—H21	119.5
C13—N2—Cu1	112.75 (14)	C22—C21—H21	119.5
C2—C1—H1A	109.5	C28—C22—C23	116.0 (2)
C2—C1—H1B	109.5	C28—C22—C21	119.6 (2)
H1A—C1—H1B	109.5	C23—C22—C21	124.3 (2)
C2—C1—H1C	109.5	C24—C23—C22	119.5 (2)
H1A—C1—H1C	109.5	C24—C23—H23	120.3
H1B—C1—H1C	109.5	C22—C23—H23	120.3
N2—C2—C3	120.5 (2)	C23—C24—C25	121.7 (2)
N2—C2—C1	118.8 (2)	C23—C24—H24	119.1
C3—C2—C1	120.7 (2)	C25—C24—H24	119.1
C4—C3—C2	120.1 (2)	N3—C25—C24	119.7 (2)
C4—C3—H3	120.0	N3—C25—C26	120.1 (2)
C2—C3—H3	120.0	C24—C25—C26	120.2 (2)
C3—C4—C5	120.1 (2)	C25—C26—H26A	109.5
C3—C4—H4	119.9	C25—C26—H26B	109.5
C5—C4—H4	119.9	H26A—C26—H26B	109.5
C4—C5—C13	116.8 (2)	C25—C26—H26C	109.5
C4—C5—C6	124.1 (2)	H26A—C26—H26C	109.5
C13—C5—C6	119.1 (2)	H26B—C26—H26C	109.5
C7—C6—C5	120.9 (2)	N4—C27—C19	123.75 (18)
C7—C6—H6	119.6	N4—C27—C28	116.32 (19)
C5—C6—H6	119.6	C19—C27—C28	119.81 (19)
C6—C7—C8	121.4 (2)	N3—C28—C22	124.35 (19)
C6—C7—H7	119.3	N3—C28—C27	116.23 (18)
C8—C7—H7	119.3	C22—C28—C27	119.3 (2)
C14—C8—C9	116.5 (2)	C29—N5—Cu1	173.4 (2)

C14—C8—C7	119.5 (2)	N5—C29—C30	178.3 (3)
C9—C8—C7	124.0 (2)	C29—C30—H30A	109.5
C10—C9—C8	119.9 (2)	C29—C30—H30B	109.5
C10—C9—H9	120.1	H30A—C30—H30B	109.5
C8—C9—H9	120.1	C29—C30—H30C	109.5
C9—C10—C11	120.5 (2)	H30A—C30—H30C	109.5
C9—C10—H10	119.8	H30B—C30—H30C	109.5
C11—C10—H10	119.8	N6—C31—C32	179.2 (3)
N1—C11—C10	121.0 (2)	C31—C32—H32A	109.5
N1—C11—C12	118.5 (2)	C31—C32—H32B	109.5
C10—C11—C12	120.4 (2)	H32A—C32—H32B	109.5
C11—C12—H12A	109.5	C31—C32—H32C	109.5
C11—C12—H12B	109.5	H32A—C32—H32C	109.5
H12A—C12—H12B	109.5	H32B—C32—H32C	109.5
C11—C12—H12C	109.5	N7—C33—C34	178.5 (3)
H12A—C12—H12C	109.5	C33—C34—H34A	109.5
H12B—C12—H12C	109.5	C33—C34—H34B	109.5
N2—C13—C5	122.4 (2)	H34A—C34—H34B	109.5
N2—C13—C14	118.18 (19)	C33—C34—H34C	109.5
C5—C13—C14	119.38 (19)	H34A—C34—H34C	109.5
N1—C14—C8	123.4 (2)	H34B—C34—H34C	109.5
N1—C14—C13	117.07 (18)	F1—B1—F4	111.3 (2)
C8—C14—C13	119.45 (19)	F1—B1—F3	107.7 (2)
C25—N3—C28	118.60 (19)	F4—B1—F3	109.3 (2)
C25—N3—Cu1	130.46 (16)	F1—B1—F2	110.3 (2)
C28—N3—Cu1	109.46 (13)	F4—B1—F2	109.8 (2)
C16—N4—C27	118.45 (18)	F3—B1—F2	108.5 (2)
C16—N4—Cu1	131.53 (15)	F8—B2—F6	113.5 (3)
C27—N4—Cu1	109.30 (12)	F8—B2—F5	108.5 (3)
C16—C15—H15A	109.5	F6—B2—F5	109.6 (3)
C16—C15—H15B	109.5	F8—B2—F7	106.8 (3)
H15A—C15—H15B	109.5	F6—B2—F7	108.0 (3)
C16—C15—H15C	109.5	F5—B2—F7	110.3 (3)
H15A—C15—H15C	109.5	F6B—B2B—F8B	112.7 (12)
H15B—C15—H15C	109.5	F6B—B2B—F7B	110.6 (12)
N4—C16—C17	120.81 (19)	F8B—B2B—F7B	101.0 (12)
N4—C16—C15	119.04 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*C*···F8^{i}	0.96	2.36	3.120 (3)	135
C18—H18···F5^{ii}	0.93	2.36	3.279 (3)	171
C20—H20···F8^{ii}	0.93	2.53	3.423 (3)	161
C30—H30*A*···F8	0.96	2.47	3.375 (4)	158

C30—H30*B*···F6^{iii}	0.96	2.38	3.314 (3)	165
C32—H32*B*···F7^{iv}	0.96	2.37	3.191 (3)	143

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