Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{*N*,*N*′-Bis[1-(pyridin-2-yl)ethylidene]propane-1,3-diamine}(thiocyanato-κ*N*)copper(II) tetrafluoridoborate

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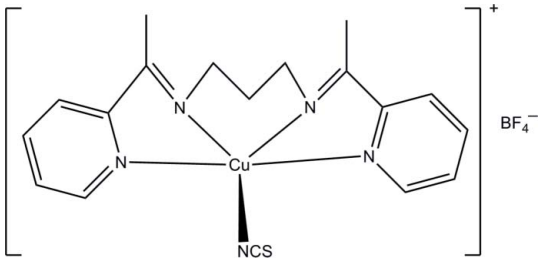
Received 30 May 2011; accepted 31 May 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.039; wR factor = 0.107; data-to-parameter ratio = 16.3.

In the title compound, $[Cu(NCS)(C_{17}H_{20}N_4)]BF_4$, the Cu^{II} ion is five-coordinated by the four N atoms of the tetradentate Schiff base ligand and one N atom of a thiocyanate ligand, thereby forming a square-pyramidal CuN_5 ccoordination geometry. The dihedral angle between the pyridine rings of the Schiff base is 55.58 (14)°. The F atoms of the tetrafluoridoborate anion are disordered over two sets of sites with occupancies of 0.614 (3) and 0.386 (3). In the crystal, the components are linked by C—H···F interactions.

Related literature

For background on the use of copper(II) complexes with Schiff bases in coordination chemistry and biological chemistry, see: Adhikary *et al.* (2009); Al-Karawi (2009); Xiao & Zhang (2009); Rajasekar *et al.* (2010); Sang & Lin (2010); Qin *et al.* (2010). For a related copper(II) complex that we reported recently, see: Liu (2010). For related copper complexes with square-pyramidal coordination, see: Liu *et al.* (1997); Chattopadhyay *et al.* (2006); Rahaman *et al.* (2005).



Experimental

Crystal data

$[Cu(NCS)(C_{17}H_{20}N_4)]BF_4$
M_r = 488.80
Monoclinic, $P2_1/c$
a = 9.5057 (7) Å
b = 13.7527 (11) Å
c = 16.1902 (13) Å
β = 101.200 (1)°
V = 2076.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 298 K
0.33 × 0.30 × 0.28 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.692, T_{max} = 0.729
17908 measured reflections
5059 independent reflections
3368 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.03
5059 reflections
310 parameters
56 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N2	1.986 (2)	Cu1—N1	2.063 (2)
Cu1—N3	2.003 (2)	Cu1—N5	2.091 (3)
Cu1—N4	2.021 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F4^{i}	0.93	2.49	3.416 (8)	176
C7—H7*B*···F4^{i}	0.96	2.34	3.234 (6)	155

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author thanks the Experimental Center of Linyi University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5899).

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supporting information

Acta Cryst. (2011). E**67**, m876–m877 [doi:10.1107/S1600536811021040]

{*N*,*N*′-Bis[1-(pyridin-2-yl)ethylidene]propane-1,3-diamine}(thiocyanato-κ*N*)copper(II) tetrafluoridoborate

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S1. Comment

Copper(II) complexes with Schiff bases have been widely investigated in coordination chemistry and biological chemistry (Adhikary *et al.*, 2009; Al-Karawi, 2009; Xiao & Zhang, 2009; Rajasekar *et al.*, 2010; Sang & Lin, 2010; Qin *et al.*, 2010). As a continuation of our work on the Schiff base copper(II) complexes (Liu, 2010), in the present paper, the title new copper complex is reported.

The title compound contains a mononuclear copper(II) complex cation and a disordered fluoroborate anion, Fig. 1. The Cu^{II} atom in the complex is five-coordinated by the four N atoms of the Schiff base ligand, and by one N atom of a thiocyanate ligand, forming a square-pyramidal geometry. The bond lengths (Table 1) related to the Cu atom are comparable with those observed in similar copper complexes with square-pyramidal geometry (Liu *et al.*, 1997; Chattopadhyay *et al.*, 2006; Rahaman *et al.*, 2005).

S2. Experimental

2-Acetylpyridine (0.2 mmol, 24.2 mg), propane-1,3-diamine (0.1 mmol, 7.4 mg), ammonium thiocyanate (0.1 mmol, 7.6 mg), copper acetate (0.1 mmol, 19.9 mg), and ammonium fluoroborate (0.1 mmol, 10.5 mg) were mixed and stirred in methanol (20 ml) at reflux for 2 h, to give a blue solution. The solution was cooled to room temperature, and blue block-shaped single crystals were formed by slow evaporation of the solution in air.

S3. Refinement

H atoms were positioned geometrically (C–H = 0.93–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C_{methyl}). The fluoroborate anion is disordered over two sites, with occupancies of 0.614 (3) and 0.386 (3).

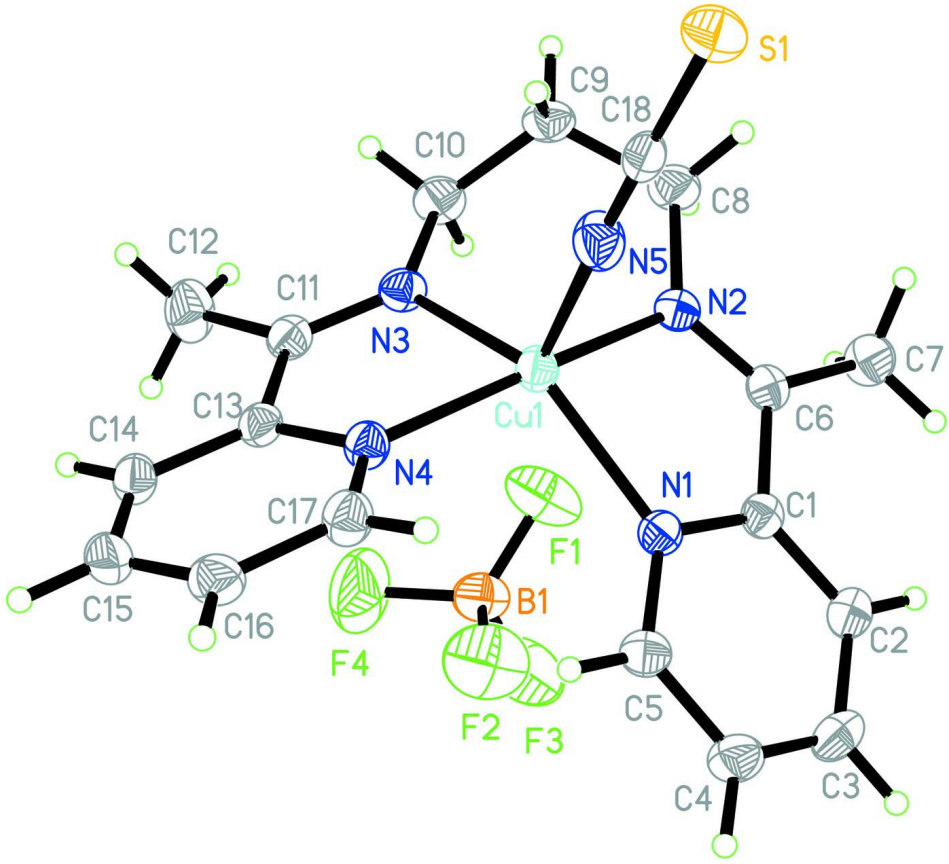

Figure 1

The molecular structure of the title complex with 30% probability displacement ellipsoids. Only the major component of the disordered fluoroborate group is shown.

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$c = 16.1902$ (13) Å
$\beta = 101.200$ (1)°
$V = 2076.2$ (3) Å^3
$Z = 4$
$F(000) = 996$
$D_x = 1.564$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4043 reflections
$\theta = 2.5$–25.1°
$\mu = 1.20$ mm^{-1}
$T = 298$ K
Block, blue
0.33 × 0.30 × 0.28 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.692$, $T_{max} = 0.729$
17908 measured reflections
5059 independent reflections
3368 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -10 \rightarrow 12$
$k = -18 \rightarrow 18$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 1.03$
5059 reflections
310 parameters
56 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
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.3601P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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	0.86559 (4)	0.35520 (2)	0.20844 (2)	0.04286 (12)	
S1	1.20466 (9)	0.30423 (6)	0.02388 (5)	0.0610 (2)	
N1	0.8455 (2)	0.22227 (15)	0.26403 (13)	0.0417 (5)	
N2	0.7105 (2)	0.29716 (16)	0.12272 (13)	0.0443 (5)	
N3	0.7727 (2)	0.48651 (16)	0.19522 (13)	0.0445 (5)	
N4	0.9890 (2)	0.42656 (15)	0.30527 (13)	0.0431 (5)	
N5	1.0234 (3)	0.33564 (18)	0.13614 (17)	0.0594 (7)	
C1	0.7394 (3)	0.16805 (18)	0.21868 (16)	0.0409 (6)	
C2	0.7017 (3)	0.0789 (2)	0.24686 (18)	0.0506 (7)	
H2	0.6281	0.0427	0.2149	0.061*	
C3	0.7750 (4)	0.0439 (2)	0.3233 (2)	0.0594 (8)	
H3	0.7513	−0.0160	0.3435	0.071*	
C4	0.8819 (4)	0.0983 (2)	0.36833 (19)	0.0593 (8)	
H4	0.9333	0.0757	0.4195	0.071*	
C5	0.9139 (3)	0.1878 (2)	0.33747 (18)	0.0523 (7)	
H5	0.9861	0.2253	0.3694	0.063*	
C6	0.6669 (3)	0.21236 (19)	0.13808 (16)	0.0424 (6)	
C7	0.5498 (3)	0.1593 (2)	0.0812 (2)	0.0595 (8)	
H7A	0.4592	0.1888	0.0838	0.089*	
H7B	0.5491	0.0926	0.0986	0.089*	
H7C	0.5656	0.1623	0.0244	0.089*	
C8	0.6416 (4)	0.3483 (2)	0.04519 (18)	0.0578 (8)	
H8A	0.5383	0.3446	0.0393	0.069*	
H8B	0.6676	0.3166	−0.0032	0.069*	
C9	0.6869 (3)	0.4539 (2)	0.04699 (17)	0.0540 (7)	

H9A	0.7885	0.4569	0.0459	0.065*	
H9B	0.6358	0.4856	−0.0035	0.065*	
C10	0.6597 (3)	0.5092 (2)	0.12256 (17)	0.0572 (8)	
H10A	0.6588	0.5785	0.1112	0.069*	
H10B	0.5670	0.4912	0.1345	0.069*	
C11	0.8076 (3)	0.54422 (19)	0.25782 (17)	0.0455 (6)	
C12	0.7350 (4)	0.6387 (2)	0.2680 (2)	0.0727 (10)	
H12A	0.7947	0.6915	0.2568	0.109*	
H12B	0.7187	0.6439	0.3245	0.109*	
H12C	0.6448	0.6414	0.2291	0.109*	
C13	0.9330 (3)	0.51342 (18)	0.32143 (16)	0.0421 (6)	
C14	0.9964 (3)	0.5691 (2)	0.38931 (17)	0.0520 (7)	
H14	0.9556	0.6280	0.4002	0.062*	
C15	1.1200 (3)	0.5373 (2)	0.44084 (18)	0.0569 (8)	
H15	1.1627	0.5738	0.4874	0.068*	
C16	1.1795 (3)	0.4511 (2)	0.42266 (18)	0.0564 (8)	
H16	1.2640	0.4286	0.4560	0.068*	
C17	1.1114 (3)	0.3979 (2)	0.35371 (19)	0.0526 (7)	
H17	1.1529	0.3401	0.3408	0.063*	
C18	1.0978 (3)	0.32353 (18)	0.08884 (17)	0.0418 (6)	
B1	0.5510 (4)	0.3543 (3)	0.3428 (2)	0.0678 (11)	0.614 (8)
F1	0.5253 (15)	0.3475 (8)	0.2600 (4)	0.138 (4)	0.614 (8)
F2	0.6776 (6)	0.3143 (6)	0.3830 (3)	0.130 (3)	0.614 (8)
F3	0.4436 (7)	0.3062 (7)	0.3717 (3)	0.140 (3)	0.614 (8)
F4	0.5594 (10)	0.4452 (3)	0.3778 (4)	0.153 (3)	0.614 (8)
B1′	0.5510 (4)	0.3543 (3)	0.3428 (2)	0.0678 (11)	0.386 (8)
F1′	0.527 (2)	0.3819 (11)	0.2591 (5)	0.116 (4)	0.386 (8)
F2′	0.5547 (12)	0.2555 (4)	0.3521 (5)	0.110 (3)	0.386 (8)
F3′	0.4465 (10)	0.3895 (9)	0.3752 (5)	0.112 (4)	0.386 (8)
F4′	0.6822 (10)	0.3896 (10)	0.3720 (6)	0.140 (5)	0.386 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0456 (2)	0.03860 (18)	0.0420 (2)	0.00179 (14)	0.00258 (14)	−0.00137 (13)
S1	0.0590 (5)	0.0726 (5)	0.0545 (5)	0.0038 (4)	0.0188 (4)	0.0015 (4)
N1	0.0429 (13)	0.0401 (11)	0.0416 (12)	0.0034 (10)	0.0073 (10)	0.0000 (9)
N2	0.0466 (14)	0.0464 (13)	0.0386 (12)	0.0007 (10)	0.0055 (10)	0.0018 (10)
N3	0.0445 (13)	0.0446 (12)	0.0440 (12)	0.0077 (10)	0.0078 (10)	0.0055 (10)
N4	0.0427 (13)	0.0398 (11)	0.0458 (12)	0.0009 (10)	0.0059 (10)	−0.0008 (9)
N5	0.0611 (17)	0.0551 (15)	0.0660 (17)	−0.0031 (13)	0.0226 (15)	−0.0104 (13)
C1	0.0391 (15)	0.0404 (14)	0.0455 (15)	0.0049 (11)	0.0141 (12)	−0.0029 (11)
C2	0.0499 (17)	0.0439 (15)	0.0594 (18)	−0.0006 (13)	0.0140 (14)	−0.0017 (13)
C3	0.066 (2)	0.0422 (16)	0.072 (2)	0.0067 (15)	0.0195 (17)	0.0127 (15)
C4	0.066 (2)	0.0563 (18)	0.0538 (18)	0.0100 (16)	0.0063 (15)	0.0111 (14)
C5	0.0571 (19)	0.0519 (16)	0.0443 (15)	0.0035 (14)	0.0012 (13)	0.0039 (13)
C6	0.0376 (15)	0.0458 (15)	0.0449 (15)	0.0022 (12)	0.0109 (12)	−0.0044 (12)
C7	0.0503 (19)	0.0624 (19)	0.0613 (19)	−0.0083 (15)	−0.0005 (15)	0.0012 (15)

C8	0.059 (2)	0.0634 (19)	0.0449 (16)	−0.0037 (15)	−0.0039 (14)	0.0073 (14)
C9	0.0571 (19)	0.0591 (18)	0.0427 (15)	0.0018 (14)	0.0020 (13)	0.0125 (13)
C10	0.0585 (19)	0.0557 (17)	0.0535 (17)	0.0154 (15)	0.0006 (15)	0.0094 (14)
C11	0.0482 (16)	0.0412 (14)	0.0502 (16)	0.0020 (12)	0.0171 (13)	0.0019 (12)
C12	0.077 (2)	0.0548 (19)	0.084 (2)	0.0179 (17)	0.009 (2)	−0.0135 (17)
C13	0.0466 (16)	0.0378 (13)	0.0450 (14)	−0.0036 (11)	0.0163 (12)	−0.0003 (11)
C14	0.065 (2)	0.0424 (14)	0.0514 (17)	−0.0083 (14)	0.0187 (15)	−0.0076 (13)
C15	0.066 (2)	0.0581 (18)	0.0460 (16)	−0.0184 (16)	0.0084 (15)	−0.0048 (14)
C16	0.0533 (18)	0.0627 (19)	0.0493 (16)	−0.0093 (15)	0.0002 (14)	0.0076 (14)
C17	0.0503 (18)	0.0466 (15)	0.0583 (18)	0.0014 (13)	0.0039 (14)	−0.0017 (13)
C18	0.0446 (16)	0.0311 (12)	0.0472 (15)	−0.0029 (11)	0.0025 (13)	0.0000 (11)
B1	0.072 (3)	0.071 (3)	0.064 (3)	0.023 (2)	0.021 (2)	0.008 (2)
F1	0.180 (6)	0.172 (8)	0.065 (4)	−0.003 (6)	0.029 (4)	−0.006 (3)
F2	0.109 (5)	0.147 (6)	0.138 (4)	0.076 (5)	0.034 (4)	0.016 (4)
F3	0.116 (5)	0.208 (8)	0.098 (3)	−0.066 (6)	0.027 (3)	−0.015 (4)
F4	0.190 (7)	0.075 (3)	0.175 (5)	0.035 (4)	−0.011 (4)	−0.017 (3)
B1′	0.072 (3)	0.071 (3)	0.064 (3)	0.023 (2)	0.021 (2)	0.008 (2)
F1′	0.142 (7)	0.129 (8)	0.084 (7)	0.010 (6)	0.038 (5)	0.041 (5)
F2′	0.128 (7)	0.077 (4)	0.122 (5)	0.005 (4)	0.013 (5)	0.011 (4)
F3′	0.111 (7)	0.145 (7)	0.094 (5)	0.073 (6)	0.059 (4)	0.020 (5)
F4′	0.114 (7)	0.169 (8)	0.127 (6)	−0.055 (7)	0.001 (5)	0.000 (6)

Geometric parameters (Å, º)

Cu1—N2	1.986 (2)	C7—H7C	0.9600
Cu1—N3	2.003 (2)	C8—C9	1.513 (4)
Cu1—N4	2.021 (2)	C8—H8A	0.9700
Cu1—N1	2.063 (2)	C8—H8B	0.9700
Cu1—N5	2.091 (3)	C9—C10	1.505 (4)
S1—C18	1.620 (3)	C9—H9A	0.9700
N1—C5	1.327 (3)	C9—H9B	0.9700
N1—C1	1.351 (3)	C10—H10A	0.9700
N2—C6	1.278 (3)	C10—H10B	0.9700
N2—C8	1.477 (3)	C11—C13	1.478 (4)
N3—C11	1.279 (3)	C11—C12	1.496 (4)
N3—C10	1.464 (3)	C12—H12A	0.9600
N4—C17	1.330 (3)	C12—H12B	0.9600
N4—C13	1.354 (3)	C12—H12C	0.9600
N5—C18	1.151 (4)	C13—C14	1.378 (4)
C1—C2	1.380 (4)	C14—C15	1.373 (4)
C1—C6	1.483 (4)	C14—H14	0.9300
C2—C3	1.383 (4)	C15—C16	1.371 (4)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.355 (4)	C16—C17	1.385 (4)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.385 (4)	C17—H17	0.9300
C4—H4	0.9300	B1—F1	1.320 (7)
C5—H5	0.9300	B1—F2	1.367 (5)

C6—C7	1.491 (4)	B1—F4	1.368 (5)
C7—H7A	0.9600	B1—F3	1.372 (5)
C7—H7B	0.9600		

N2—Cu1—N3	92.05 (9)	N2—C8—H8A	109.4
N2—Cu1—N4	167.96 (9)	C9—C8—H8A	109.4
N3—Cu1—N4	79.77 (9)	N2—C8—H8B	109.4
N2—Cu1—N1	80.19 (9)	C9—C8—H8B	109.4
N3—Cu1—N1	140.31 (9)	H8A—C8—H8B	108.0
N4—Cu1—N1	100.42 (8)	C10—C9—C8	114.0 (3)
N2—Cu1—N5	94.19 (10)	C10—C9—H9A	108.7
N3—Cu1—N5	113.90 (9)	C8—C9—H9A	108.7
N4—Cu1—N5	97.20 (9)	C10—C9—H9B	108.7
N1—Cu1—N5	105.51 (9)	C8—C9—H9B	108.7
C5—N1—C1	118.3 (2)	H9A—C9—H9B	107.6
C5—N1—Cu1	129.53 (19)	N3—C10—C9	109.3 (2)
C1—N1—Cu1	112.00 (17)	N3—C10—H10A	109.8
C6—N2—C8	119.6 (2)	C9—C10—H10A	109.8
C6—N2—Cu1	117.11 (18)	N3—C10—H10B	109.8
C8—N2—Cu1	123.28 (18)	C9—C10—H10B	109.8
C11—N3—C10	122.8 (2)	H10A—C10—H10B	108.3
C11—N3—Cu1	115.70 (18)	N3—C11—C13	115.1 (2)
C10—N3—Cu1	121.13 (18)	N3—C11—C12	124.9 (3)
C17—N4—C13	118.6 (2)	C13—C11—C12	120.0 (3)
C17—N4—Cu1	128.55 (19)	C11—C12—H12A	109.5
C13—N4—Cu1	112.82 (17)	C11—C12—H12B	109.5
C18—N5—Cu1	172.4 (3)	H12A—C12—H12B	109.5
N1—C1—C2	121.7 (2)	C11—C12—H12C	109.5
N1—C1—C6	115.0 (2)	H12A—C12—H12C	109.5
C2—C1—C6	123.3 (3)	H12B—C12—H12C	109.5
C1—C2—C3	119.1 (3)	N4—C13—C14	121.1 (3)
C1—C2—H2	120.4	N4—C13—C11	114.3 (2)
C3—C2—H2	120.4	C14—C13—C11	124.4 (2)
C4—C3—C2	119.0 (3)	C15—C14—C13	119.8 (3)
C4—C3—H3	120.5	C15—C14—H14	120.1
C2—C3—H3	120.5	C13—C14—H14	120.1
C3—C4—C5	119.4 (3)	C16—C15—C14	119.0 (3)
C3—C4—H4	120.3	C16—C15—H15	120.5
C5—C4—H4	120.3	C14—C15—H15	120.5
N1—C5—C4	122.5 (3)	C15—C16—C17	118.8 (3)
N1—C5—H5	118.8	C15—C16—H16	120.6
C4—C5—H5	118.8	C17—C16—H16	120.6
N2—C6—C1	115.7 (2)	N4—C17—C16	122.5 (3)
N2—C6—C7	123.9 (2)	N4—C17—H17	118.8
C1—C6—C7	120.4 (2)	C16—C17—H17	118.8
C6—C7—H7A	109.5	N5—C18—S1	178.5 (3)
C6—C7—H7B	109.5	F1—B1—F2	115.3 (7)
H7A—C7—H7B	109.5	F1—B1—F4	118.0 (6)

C6—C7—H7C	109.5	F2—B1—F4	101.3 (5)
H7A—C7—H7C	109.5	F1—B1—F3	108.0 (7)
H7B—C7—H7C	109.5	F2—B1—F3	106.8 (5)
N2—C8—C9	111.3 (2)	F4—B1—F3	106.7 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···F4^{i}	0.93	2.49	3.416 (8)	176
C7—H7*B*···F4^{i}	0.96	2.34	3.234 (6)	155

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+1/2.