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catena-Poly[[copper(I)-μ-2,6-bis[4-(pyridin-2-yl)thiazol-2-yl]pyridine] hexafluoridophosphate acetonitrile monosolvate] from single-crystal synchrotron data

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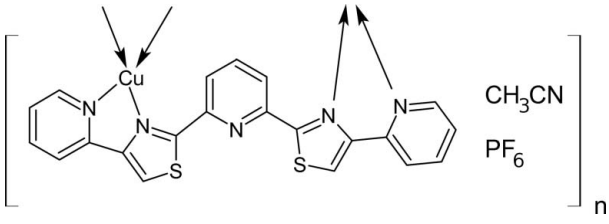
Key indicators: single-crystal synchrotron study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.031; wR factor = 0.078; data-to-parameter ratio = 10.0.

The title complex, $\{[Cu(C_{21}H_{13}N_5S_2)]PF_6\cdot CH_3CN\}_n$, was formed immediately on adding together a methanol solution containing copper(I) ions and a methanol solution of 2,6-bis[4-(pyridin-2-yl)thiazol-2-yl]pyridine. Crystallographic studies of the complex reveal a coordination polymer with the ligand acting as a bis(bidentate) ligand with the pyridine N atom not coordinating a metal centre. The Cu^I atom is four-coordinate with approximately tetrahedral stereochemistry: the N_4 donor set is provided by bipyridine-like moieties of the two heterocyclic ligands. Parallel chains of the coordination polymer run along the b-axis direction with the disordered (0.50:0.50 occupancy ratio) PF_6^- anions and acetonitrile solvent molecules located between the chains.

Related literature

For a related complex, see: Baker & Matthews (1999).



Experimental

Crystal data

$[Cu(C_{21}H_{13}N_5S_2)]PF_6\cdot C_2H_3N$
M_r = 649.05
Monoclinic, $P2_1/c$
a = 12.525 (3) Å
b = 13.950 (3) Å
c = 14.626 (3) Å
β = 97.72 (3)°
V = 2532.4 (9) Å^3
Z = 4
Synchrotron radiation
λ = 0.71073 Å
μ = 1.16 mm^{-1}
T = 100 K
0.03 × 0.02 × 0.01 mm

Data collection

3-BM1 Australian Synchrotron diffractometer
28022 measured reflections
3890 independent reflections
3641 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 23.8°

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.08
3890 reflections
389 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Data collection: *BLU-ICE* (McPhillips *et al.*, 2002); cell refinement: *XDS* (Kabsch, 1993); data reduction: *XDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2190).

References

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supplementary materials

Acta Cryst. (2013). E**69**, m231 [doi:10.1107/S1600536813006831]

catena-Poly[[copper(I)-μ-2,6-bis[4-(pyridin-2-yl)thiazol-2-yl]pyridine] hexafluoridophosphate acetonitrile monosolvate] from single-crystal synchrotron data

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Comment

We have prepared and studied many analogues of 2,2′-bipyridine and 2,2′:6′,2"-terpyridine (Baker and Matthews, 1999 and references therein) and have extended this work to the preparation of ligands analogous to quinquepyridine. For metal complexes of these quinquepyridine analogues, a number of features have been observed. The interpolation of a five-membered heterocycle appears to reduce the capacity of the ligands to employ all five donor atoms and we have seen several examples where the ligands act in a bis(bidentate) mode [2 + 2]. In such cases the ligands bridge between metal centres in binuclear complexes. Herein we report a coordination polymer shown in Scheme 1, again where the ligand binds in [2 + 2] mode. A thermal ellipsoid plot is shown in Fig. 1. Each copper centre has approximately tetrahedral stereochemistry as shown in Fig. 1. The principal cause of distortion being the bite angles of the bidentate ligand N2B—Cu1—N1B (82.47 (8)°) and N2A^{i}—Cu1—N1A^{i} (82.95 (8)°) (symmetry code: (i) -*x* + 1, *y* + 1/2, -*z* + 1/2) are considerably less than the ideal tetrahedral angle. Two 'thiazolylpyridine′ moieties coordinate each copper(I) centre with the relevant bond lengths being Cu—N1A^{i} 2.098 (2) Å, Cu—N1B 2.050 (2) Å, Cu—N2A 1.992 (2) Å and Cu—N2B 2.024 (2) Å. The Cu—N bond lengths are similar but the Cu—$N_{pyridinyl}$ bonds are slightly shorter than the Cu—$N_{thiazolyl}$ bonds. This indicates a slightly stronger interaction of the metal atom with the pyridinyl moiety, in line with base strength. A single chain of the coordination polymer, thus created, is depicted in Fig. 2 and packing of these chains that include PF_6^- anions and solvent molecules of acetonitriles are shown in Fig. 3.

Experimental

The quinquedentate ligand 2,6-bis(4-(pyridin-2-yl)thiazol-2-yl)pyridine was prepared by adding a solution of 2-(bromo-acetyl)pyridinium hydrobromide (5.6 g, 20 mmol) in hot ethanol (50 ml) to a solution of 2,6-di(thioamido)pyridine (2.0 g, 10 mmol) in hot ethanol (50 ml). The solution was heated for 5 min, a yellow precipitate of 2,6-bis(4-(pyridin-2-yl)thiazol-2-yl)pyridinium hydrobromide separated soon. The mixture was allowed to stand for 30 min s and the yellow precipitate was filtered and washed with sodium bicarbonate (5%) until effervescence ceased. Yield: 75%. The complex was prepared as follows: Tetrakis(acetonitrile)copper(I) hexafluorophosphate (200 mg, 0.54 mmol) in hot methanol (20 ml) was added to a solution of the ligand (214 mg, 0.54 mmol) in hot methanol (20 ml). The reaction mixture was heated on the water bath for 1 h. An orange solid formed during this time and once cooled the solid was collected, washed with cooled methanol and stored over silica gel (yield 164 mg, 50%). Crystals were grown by vapour diffusion of diethyl ether into a concentrated acetonitrile solution of the complex.

Refinement

All the H-atoms were fixed stereochemically and included in the refinement using riding model option in *SHELXL97*. The PF6 anion was found to exhibit orientational disorder, which was modelled over two positions.

H atoms were positioned geometrically with C—H = 0.93 - 0.96 Å. U_{iso}(H) values were set at 1.2U_{eq} (aromatic) or 1.5U_{eq} of the parent atom (methyl group).

Computing details

Data collection: BLU-ICE (McPhillips *et al.*, 2002); cell refinement: XDS (Kabsch, 1993); data reduction: XDS (Kabsch, 1993); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

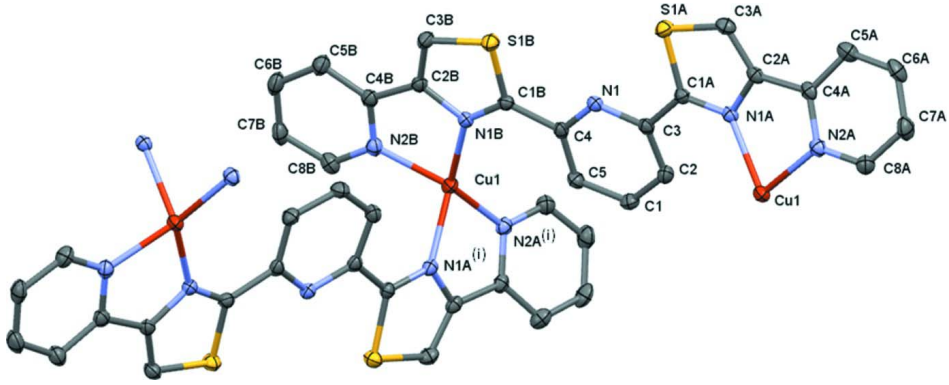

Figure 1

Thermal ellipsoids plot (40% probability) of the part of the coordination polymer showing the geometry around Cu(I) ion. Hydrogen atoms, the PF_6 anion and the solvent acetonitrile molecule are omitted for clarity. Symmetry code: (i) -*x* + 1, *y* + 1/2, -*z* + 1/2.

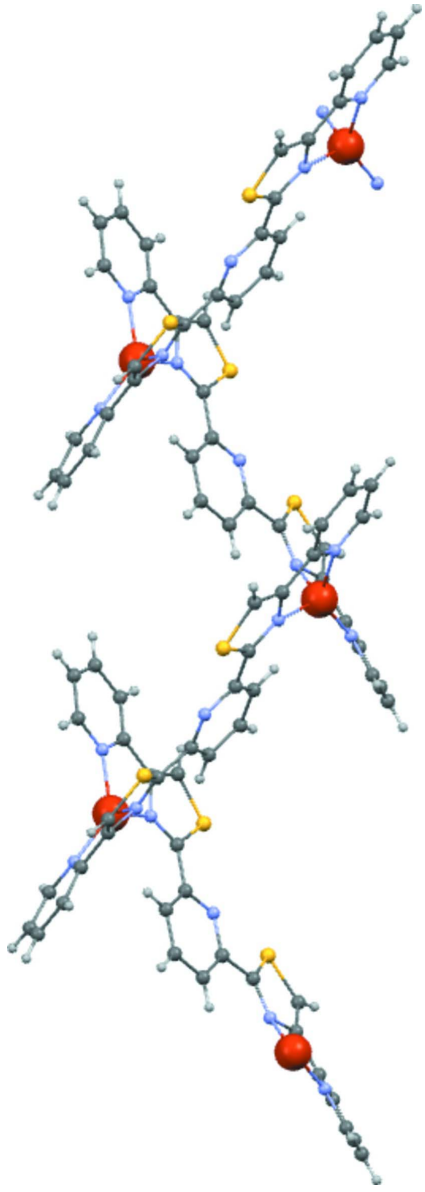

Figure 2

A single chain showing the construction of the coordination polymer formed with the ligand.

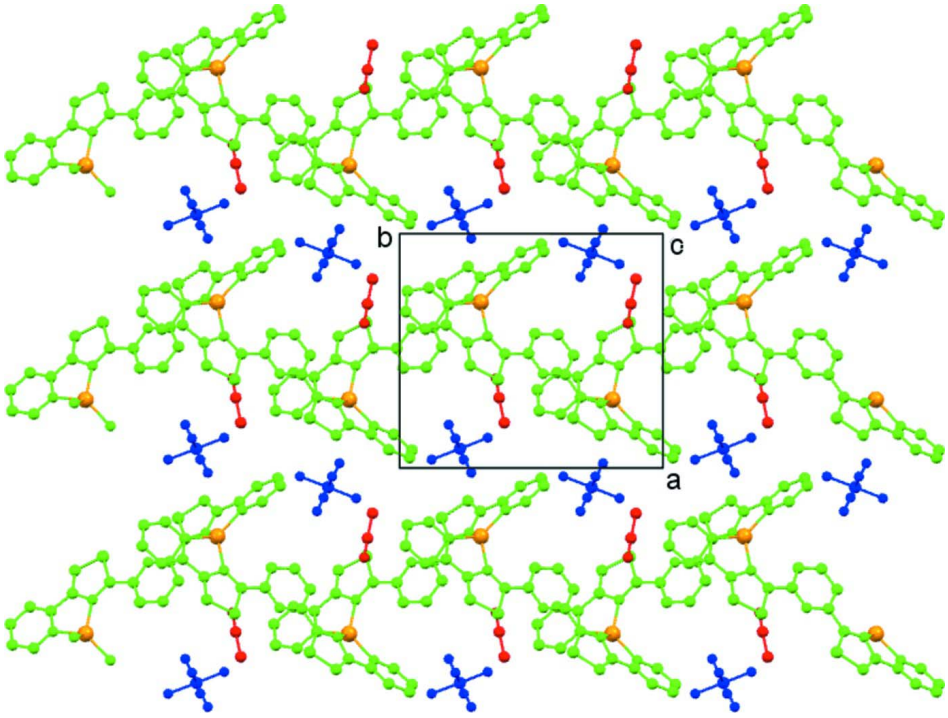

Figure 3

Packing of coordination polymers viewed down *c* axis that includes PF6 anions (disorder omitted for clarity) and solvent molecules (acetonitrile).

catena-Poly[[copper(I)-*μ*-2,6-bis[4-(pyridin-2-yl)thiazol-2-yl]pyridine] hexafluoridophosphate acetonitrile monosolvate]

Crystal data

$[Cu(C_{21}H_{13}N_5S_2)]PF_6 \cdot C_2H_3N$
$M_r = 649.05$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.525$ (3) Å
$b = 13.950$ (3) Å
$c = 14.626$ (3) Å
$\beta = 97.72$ (3)°
$V = 2532.4$ (9) Å^3
$Z = 4$
$F(000) = 1304$
$D_x = 1.702$ Mg m^{-3}
Synchrotron radiation, $\lambda = 0.71073$ Å
Cell parameters from 9980 reflections
$\theta = 2.5$–$22.5°$
$\mu = 1.16$ mm^{-1}
$T = 100$ K
Thin plates, blue
0.03 × 0.02 × 0.01 mm

Data collection

3-BM1 Australian Synchrotron diffractometer
Radiation source: Synchrotron BM
Si<111> monochromator
φ scans
28022 measured reflections
3890 independent reflections
3641 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 23.8°$, $\theta_{min} = 1.6°$
$h = -14 \rightarrow 14$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.078$
$S = 1.08$
3890 reflections
389 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 3.8973P]$,$P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ 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	0.70815 (2)	1.19154 (2)	0.36895 (2)	0.01965 (11)	
N1	0.40269 (16)	0.95445 (14)	0.35587 (13)	0.0159 (4)	
C1	0.5696 (2)	0.89759 (19)	0.25992 (17)	0.0211 (6)	
H1	0.6257	0.8784	0.2285	0.025*	
C2	0.4814 (2)	0.83892 (18)	0.26281 (17)	0.0197 (5)	
H2	0.4773	0.7794	0.2339	0.024*	
C3	0.3990 (2)	0.87086 (17)	0.30999 (16)	0.0165 (5)	
C4	0.48924 (19)	1.00992 (17)	0.35293 (16)	0.0162 (5)	
C5	0.5735 (2)	0.98545 (18)	0.30444 (17)	0.0197 (5)	
H5	0.6311	1.0270	0.3020	0.024*	
S1A	0.21354 (5)	0.84000 (5)	0.39190 (4)	0.02002 (16)	
N1A	0.27744 (16)	0.73513 (14)	0.26615 (14)	0.0163 (4)	
N2A	0.17898 (16)	0.59744 (15)	0.15433 (14)	0.0180 (4)	
C1A	0.3024 (2)	0.81261 (17)	0.31486 (16)	0.0160 (5)	
C2A	0.18499 (19)	0.69316 (17)	0.28980 (17)	0.0173 (5)	
C3A	0.1400 (2)	0.74016 (19)	0.35688 (17)	0.0207 (5)	
H3A	0.0781	0.7207	0.3803	0.025*	
C4A	0.14469 (19)	0.60735 (18)	0.23785 (17)	0.0173 (5)	
C5A	0.0784 (2)	0.5404 (2)	0.27187 (18)	0.0239 (6)	
H5A	0.0574	0.5484	0.3300	0.029*	
C6A	0.0438 (2)	0.4617 (2)	0.21859 (19)	0.0276 (6)	
H6A	−0.0001	0.4157	0.2405	0.033*	
C7A	0.0757 (2)	0.4527 (2)	0.13181 (19)	0.0275 (6)	
H7A	0.0520	0.4015	0.0937	0.033*	
C8A	0.1432 (2)	0.52119 (18)	0.10326 (18)	0.0232 (6)	
H8A	0.1652	0.5142	0.0454	0.028*	

S1B	0.37811 (5)	1.12599 (5)	0.46088 (4)	0.02089 (16)	
N1B	0.56301 (16)	1.16578 (14)	0.41446 (13)	0.0154 (4)	
N2B	0.69867 (17)	1.31538 (14)	0.43946 (14)	0.0193 (5)	
C1B	0.48752 (19)	1.09985 (18)	0.40534 (16)	0.0165 (5)	
C2B	0.5353 (2)	1.24125 (18)	0.46810 (16)	0.0173 (5)	
C3B	0.4376 (2)	1.23154 (18)	0.49859 (17)	0.0207 (5)	
H4B	0.4076	1.2762	0.5349	0.025*	
C4B	0.6105 (2)	1.32303 (18)	0.48297 (17)	0.0190 (5)	
C5B	0.5930 (2)	1.40191 (19)	0.53706 (18)	0.0248 (6)	
H5B	0.5330	1.4047	0.5682	0.030*	
C6B	0.6670 (2)	1.47623 (19)	0.54353 (19)	0.0290 (6)	
H6B	0.6566	1.5303	0.5785	0.035*	
C7B	0.7559 (2)	1.46972 (19)	0.49804 (18)	0.0263 (6)	
H7B	0.8059	1.5193	0.5013	0.032*	
C8B	0.7696 (2)	1.38795 (19)	0.44740 (18)	0.0239 (6)	
H8B	0.8305	1.3831	0.4176	0.029*	
P1	0.91781 (5)	0.77051 (5)	0.06197 (5)	0.02250 (17)	
F1	1.02028 (15)	0.72763 (13)	0.02232 (14)	0.0467 (5)	
F2	0.9637 (5)	0.7561 (5)	0.1692 (5)	0.0320 (13)	0.50
F3	0.8706 (11)	0.6650 (9)	0.0595 (7)	0.034 (2)	0.50
F4	0.8738 (5)	0.7876 (5)	−0.0432 (4)	0.0503 (15)	0.50
F5	0.9640 (8)	0.8778 (6)	0.0694 (4)	0.0348 (15)	0.50
F2′	1.0012 (6)	0.7796 (6)	0.1511 (5)	0.064 (2)	0.50
F3′	0.8878 (13)	0.6654 (11)	0.0896 (8)	0.063 (4)	0.50
F4′	0.8345 (5)	0.7575 (6)	−0.0299 (5)	0.063 (2)	0.50
F5′	0.9533 (8)	0.8721 (7)	0.0272 (6)	0.080 (3)	0.50
F6	0.81523 (16)	0.81302 (15)	0.10063 (17)	0.0572 (6)	
C1AN	0.1934 (3)	0.1022 (3)	0.2238 (2)	0.0507 (9)	
H1A1	0.1468	0.0772	0.1718	0.076*	
H1A2	0.1637	0.1606	0.2442	0.076*	
H1A3	0.2001	0.0562	0.2730	0.076*	
C2AN	0.2998 (3)	0.1214 (2)	0.19694 (19)	0.0297 (7)	
N1AN	0.3824 (2)	0.13309 (19)	0.17597 (18)	0.0368 (6)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02253 (19)	0.01556 (18)	0.02245 (18)	0.00197 (12)	0.00884 (13)	−0.00093 (12)
N1	0.0184 (11)	0.0143 (10)	0.0151 (10)	0.0000 (8)	0.0026 (8)	0.0017 (8)
C1	0.0218 (13)	0.0219 (14)	0.0209 (13)	0.0003 (11)	0.0083 (10)	−0.0021 (11)
C2	0.0243 (14)	0.0154 (13)	0.0195 (13)	−0.0016 (10)	0.0031 (10)	−0.0016 (10)
C3	0.0198 (13)	0.0146 (12)	0.0146 (12)	0.0000 (10)	0.0012 (10)	0.0032 (10)
C4	0.0214 (13)	0.0130 (12)	0.0137 (12)	−0.0013 (10)	0.0000 (10)	0.0016 (10)
C5	0.0195 (13)	0.0194 (13)	0.0210 (13)	−0.0038 (10)	0.0058 (10)	0.0006 (10)
S1A	0.0198 (3)	0.0213 (3)	0.0196 (3)	0.0006 (3)	0.0054 (2)	−0.0028 (3)
N1A	0.0173 (10)	0.0145 (11)	0.0172 (10)	0.0002 (8)	0.0024 (8)	0.0026 (9)
N2A	0.0174 (10)	0.0165 (11)	0.0199 (11)	0.0017 (9)	0.0022 (8)	0.0025 (9)
C1A	0.0179 (12)	0.0151 (13)	0.0150 (12)	0.0023 (10)	0.0025 (10)	0.0023 (10)
C2A	0.0157 (12)	0.0173 (13)	0.0188 (12)	0.0003 (10)	0.0016 (10)	0.0047 (10)
C3A	0.0173 (13)	0.0243 (14)	0.0211 (13)	−0.0019 (11)	0.0046 (10)	0.0023 (11)

C4A	0.0148 (12)	0.0160 (13)	0.0207 (13)	0.0019 (10)	0.0009 (10)	0.0041 (10)
C5A	0.0221 (14)	0.0262 (14)	0.0233 (13)	−0.0032 (11)	0.0029 (11)	0.0052 (11)
C6A	0.0258 (14)	0.0227 (14)	0.0337 (15)	−0.0093 (11)	0.0023 (12)	0.0069 (12)
C7A	0.0317 (15)	0.0188 (14)	0.0310 (15)	−0.0073 (12)	0.0004 (12)	−0.0022 (12)
C8A	0.0272 (14)	0.0199 (14)	0.0226 (13)	−0.0005 (11)	0.0036 (11)	−0.0002 (11)
S1B	0.0197 (3)	0.0201 (3)	0.0244 (3)	−0.0023 (3)	0.0085 (3)	−0.0034 (3)
N1B	0.0189 (11)	0.0132 (10)	0.0146 (10)	0.0000 (8)	0.0038 (8)	0.0009 (8)
N2B	0.0225 (11)	0.0152 (11)	0.0197 (11)	0.0005 (9)	0.0010 (9)	0.0010 (9)
C1B	0.0181 (12)	0.0178 (13)	0.0141 (12)	0.0018 (10)	0.0039 (10)	0.0021 (10)
C2B	0.0230 (13)	0.0148 (12)	0.0142 (12)	0.0020 (10)	0.0025 (10)	0.0001 (10)
C3B	0.0231 (14)	0.0186 (13)	0.0212 (13)	0.0005 (11)	0.0059 (10)	−0.0051 (11)
C4B	0.0229 (13)	0.0166 (13)	0.0172 (12)	0.0019 (10)	0.0013 (10)	0.0019 (10)
C5B	0.0294 (15)	0.0196 (14)	0.0253 (14)	0.0035 (11)	0.0037 (11)	−0.0033 (11)
C6B	0.0404 (17)	0.0173 (14)	0.0288 (15)	0.0022 (12)	0.0022 (13)	−0.0060 (11)
C7B	0.0336 (16)	0.0153 (13)	0.0283 (15)	−0.0057 (11)	−0.0021 (12)	−0.0008 (11)
C8B	0.0236 (14)	0.0212 (14)	0.0269 (14)	−0.0031 (11)	0.0030 (11)	0.0038 (11)
P1	0.0214 (4)	0.0218 (4)	0.0244 (4)	0.0027 (3)	0.0035 (3)	0.0035 (3)
F1	0.0402 (11)	0.0389 (11)	0.0688 (13)	0.0088 (8)	0.0354 (10)	0.0116 (9)
F2	0.046 (4)	0.029 (2)	0.021 (2)	0.009 (2)	0.003 (2)	0.0040 (16)
F3	0.033 (4)	0.020 (4)	0.051 (5)	−0.010 (3)	0.016 (3)	−0.016 (4)
F4	0.064 (5)	0.061 (4)	0.023 (2)	0.018 (3)	−0.008 (3)	0.011 (2)
F5	0.046 (3)	0.017 (2)	0.046 (3)	−0.001 (2)	0.024 (3)	−0.002 (3)
F2′	0.053 (5)	0.092 (6)	0.039 (4)	0.035 (4)	−0.018 (3)	−0.038 (4)
F3′	0.051 (6)	0.043 (5)	0.103 (10)	0.004 (4)	0.037 (6)	0.032 (6)
F4′	0.031 (3)	0.113 (6)	0.041 (3)	0.001 (3)	−0.010 (2)	0.001 (3)
F5′	0.038 (3)	0.030 (4)	0.176 (9)	0.006 (3)	0.027 (6)	0.054 (6)
F6	0.0392 (11)	0.0510 (13)	0.0864 (16)	0.0157 (9)	0.0267 (11)	−0.0079 (11)
C1AN	0.0362 (19)	0.077 (3)	0.0421 (19)	−0.0020 (18)	0.0159 (15)	0.0064 (19)
C2AN	0.0368 (18)	0.0305 (16)	0.0215 (14)	0.0006 (13)	0.0026 (13)	0.0061 (12)
N1AN	0.0347 (16)	0.0418 (16)	0.0340 (14)	−0.0042 (12)	0.0049 (12)	0.0149 (12)

Geometric parameters (Å, º)

Cu1—N2A^{i}	1.992 (2)	C8A—H8A	0.9300
Cu1—N2B	2.024 (2)	S1B—C3B	1.708 (3)
Cu1—N1B	2.050 (2)	S1B—C1B	1.723 (2)
Cu1—N1A^{i}	2.098 (2)	N1B—C1B	1.313 (3)
N1—C4	1.337 (3)	N1B—C2B	1.385 (3)
N1—C3	1.343 (3)	N2B—C8B	1.342 (3)
C1—C2	1.380 (4)	N2B—C4B	1.351 (3)
C1—C5	1.386 (4)	C2B—C3B	1.364 (4)
C1—H1	0.9300	C2B—C4B	1.476 (4)
C2—C3	1.390 (4)	C3B—H4B	0.9300
C2—H2	0.9300	C4B—C5B	1.390 (4)
C3—C1A	1.467 (3)	C5B—C6B	1.385 (4)
C4—C5	1.391 (4)	C5B—H5B	0.9300
C4—C1B	1.472 (3)	C6B—C7B	1.375 (4)
C5—H5	0.9300	C6B—H6B	0.9300
S1A—C3A	1.710 (3)	C7B—C8B	1.383 (4)
S1A—C1A	1.730 (2)	C7B—H7B	0.9300

N1A—C1A	1.309 (3)	C8B—H8B	0.9300
N1A—C2A	1.382 (3)	P1—F2′	1.562 (7)
N1A—Cu1^{ii}	2.098 (2)	P1—F3′	1.580 (16)
N2A—C8A	1.342 (3)	P1—F4	1.581 (6)
N2A—C4A	1.355 (3)	P1—F3	1.585 (13)
N2A—Cu1^{ii}	1.992 (2)	P1—F6	1.587 (2)
C2A—C3A	1.363 (4)	P1—F5′	1.589 (9)
C2A—C4A	1.470 (4)	P1—F1	1.5941 (18)
C3A—H3A	0.9300	P1—F4′	1.597 (7)
C4A—C5A	1.385 (4)	P1—F5	1.603 (9)
C5A—C6A	1.382 (4)	P1—F2	1.609 (7)
C5A—H5A	0.9300	C1AN—C2AN	1.464 (4)
C6A—C7A	1.387 (4)	C1AN—H1A1	0.9600
C6A—H6A	0.9300	C1AN—H1A2	0.9600
C7A—C8A	1.377 (4)	C1AN—H1A3	0.9600
C7A—H7A	0.9300	C2AN—N1AN	1.130 (4)

N2A^{i}—Cu1—N2B	137.85 (9)	S1B—C3B—H4B	124.7
N2A^{i}—Cu1—N1B	128.37 (8)	N2B—C4B—C5B	122.1 (2)
N2B—Cu1—N1B	82.47 (8)	N2B—C4B—C2B	114.5 (2)
N2A^{i}—Cu1—N1A^{i}	82.95 (8)	C5B—C4B—C2B	123.3 (2)
N2B—Cu1—N1A^{i}	104.53 (8)	C6B—C5B—C4B	118.5 (3)
N1B—Cu1—N1A^{i}	123.28 (8)	C6B—C5B—H5B	120.8
C4—N1—C3	117.4 (2)	C4B—C5B—H5B	120.8
C2—C1—C5	119.2 (2)	C7B—C6B—C5B	119.7 (3)
C2—C1—H1	120.4	C7B—C6B—H6B	120.1
C5—C1—H1	120.4	C5B—C6B—H6B	120.1
C1—C2—C3	118.4 (2)	C6B—C7B—C8B	118.7 (3)
C1—C2—H2	120.8	C6B—C7B—H7B	120.7
C3—C2—H2	120.8	C8B—C7B—H7B	120.7
N1—C3—C2	123.3 (2)	N2B—C8B—C7B	122.7 (3)
N1—C3—C1A	115.5 (2)	N2B—C8B—H8B	118.6
C2—C3—C1A	121.3 (2)	C7B—C8B—H8B	118.6
N1—C4—C5	123.3 (2)	F2′—P1—F3′	91.0 (5)
N1—C4—C1B	114.1 (2)	F2′—P1—F4	155.0 (4)
C5—C4—C1B	122.7 (2)	F3′—P1—F4	109.0 (5)
C1—C5—C4	118.4 (2)	F2′—P1—F3	107.4 (5)
C1—C5—H5	120.8	F3′—P1—F3	16.8 (6)
C4—C5—H5	120.8	F4—P1—F3	92.2 (5)
C3A—S1A—C1A	89.57 (12)	F2′—P1—F6	98.9 (3)
C1A—N1A—C2A	111.1 (2)	F3′—P1—F6	91.4 (6)
C1A—N1A—Cu1^{ii}	135.01 (17)	F4—P1—F6	95.6 (3)
C2A—N1A—Cu1^{ii}	107.09 (15)	F3—P1—F6	92.2 (5)
C8A—N2A—C4A	117.4 (2)	F2′—P1—F5′	90.6 (5)
C8A—N2A—Cu1^{ii}	128.23 (18)	F3′—P1—F5′	174.9 (7)
C4A—N2A—Cu1^{ii}	113.89 (16)	F4—P1—F5′	68.3 (4)
N1A—C1A—C3	124.7 (2)	F3—P1—F5′	160.2 (5)
N1A—C1A—S1A	114.16 (18)	F6—P1—F5′	93.2 (3)
C3—C1A—S1A	121.09 (18)	F2′—P1—F1	81.6 (3)

C3A—C2A—N1A	114.7 (2)	F3′—P1—F1	88.6 (6)
C3A—C2A—C4A	128.1 (2)	F4—P1—F1	84.0 (3)
N1A—C2A—C4A	117.2 (2)	F3—P1—F1	87.7 (5)
C2A—C3A—S1A	110.47 (19)	F6—P1—F1	179.52 (13)
C2A—C3A—H3A	124.8	F5′—P1—F1	86.8 (3)
S1A—C3A—H3A	124.8	F2′—P1—F4′	177.9 (4)
N2A—C4A—C5A	122.2 (2)	F3′—P1—F4′	87.6 (5)
N2A—C4A—C2A	114.9 (2)	F4—P1—F4′	25.2 (2)
C5A—C4A—C2A	122.9 (2)	F3—P1—F4′	71.1 (5)
C6A—C5A—C4A	119.4 (2)	F6—P1—F4′	82.8 (3)
C6A—C5A—H5A	120.3	F5′—P1—F4′	90.7 (4)
C4A—C5A—H5A	120.3	F1—P1—F4′	96.8 (3)
C5A—C6A—C7A	118.8 (2)	F2′—P1—F5	70.9 (4)
C5A—C6A—H6A	120.6	F3′—P1—F5	161.0 (4)
C7A—C6A—H6A	120.6	F4—P1—F5	90.0 (3)
C8A—C7A—C6A	118.6 (3)	F3—P1—F5	177.2 (5)
C8A—C7A—H7A	120.7	F6—P1—F5	86.0 (3)
C6A—C7A—H7A	120.7	F5′—P1—F5	22.4 (4)
N2A—C8A—C7A	123.6 (2)	F1—P1—F5	94.2 (3)
N2A—C8A—H8A	118.2	F4′—P1—F5	110.7 (4)
C7A—C8A—H8A	118.2	F2′—P1—F2	23.9 (3)
C3B—S1B—C1B	89.68 (12)	F3′—P1—F2	72.6 (4)
C1B—N1B—C2B	111.0 (2)	F4—P1—F2	178.4 (3)
C1B—N1B—Cu1	138.40 (17)	F3—P1—F2	89.4 (4)
C2B—N1B—Cu1	110.56 (16)	F6—P1—F2	84.2 (2)
C8B—N2B—C4B	118.3 (2)	F5′—P1—F2	110.2 (4)
C8B—N2B—Cu1	127.22 (18)	F1—P1—F2	96.2 (2)
C4B—N2B—Cu1	114.53 (17)	F4′—P1—F2	156.0 (3)
N1B—C1B—C4	126.1 (2)	F5—P1—F2	88.4 (3)
N1B—C1B—S1B	114.28 (18)	C2AN—C1AN—H1A1	109.5
C4—C1B—S1B	119.61 (18)	C2AN—C1AN—H1A2	109.5
C3B—C2B—N1B	114.4 (2)	H1A1—C1AN—H1A2	109.5
C3B—C2B—C4B	127.6 (2)	C2AN—C1AN—H1A3	109.5
N1B—C2B—C4B	117.9 (2)	H1A1—C1AN—H1A3	109.5
C2B—C3B—S1B	110.60 (19)	H1A2—C1AN—H1A3	109.5
C2B—C3B—H4B	124.7	N1AN—C2AN—C1AN	177.8 (4)

C5—C1—C2—C3	0.5 (4)	N2B—Cu1—N1B—C1B	176.7 (3)
C4—N1—C3—C2	2.0 (3)	N1A^{i}—Cu1—N1B—C1B	74.2 (3)
C4—N1—C3—C1A	−179.8 (2)	N2A^{i}—Cu1—N1B—C2B	147.28 (15)
C1—C2—C3—N1	−2.6 (4)	N2B—Cu1—N1B—C2B	−0.84 (16)
C1—C2—C3—C1A	179.3 (2)	N1A^{i}—Cu1—N1B—C2B	−103.31 (16)
C3—N1—C4—C5	0.6 (3)	N2A^{i}—Cu1—N2B—C8B	39.4 (3)
C3—N1—C4—C1B	−179.6 (2)	N1B—Cu1—N2B—C8B	−178.7 (2)
C2—C1—C5—C4	1.9 (4)	N1A^{i}—Cu1—N2B—C8B	−56.2 (2)
N1—C4—C5—C1	−2.6 (4)	N2A^{i}—Cu1—N2B—C4B	−140.17 (17)
C1B—C4—C5—C1	177.7 (2)	N1B—Cu1—N2B—C4B	1.73 (17)
C2A—N1A—C1A—C3	176.6 (2)	N1A^{i}—Cu1—N2B—C4B	124.25 (17)
Cu1^{ii}—N1A—C1A—C3	−37.1 (4)	C2B—N1B—C1B—C4	179.8 (2)

C2A—N1A—C1A—S1A	−0.7 (3)	Cu1—N1B—C1B—C4	2.3 (4)
Cu1^{ii}—N1A—C1A—S1A	145.62 (16)	C2B—N1B—C1B—S1B	0.3 (3)
N1—C3—C1A—N1A	171.2 (2)	Cu1—N1B—C1B—S1B	−177.16 (14)
C2—C3—C1A—N1A	−10.5 (4)	N1—C4—C1B—N1B	179.0 (2)
N1—C3—C1A—S1A	−11.7 (3)	C5—C4—C1B—N1B	−1.2 (4)
C2—C3—C1A—S1A	166.63 (19)	N1—C4—C1B—S1B	−1.5 (3)
C3A—S1A—C1A—N1A	0.76 (19)	C5—C4—C1B—S1B	178.24 (19)
C3A—S1A—C1A—C3	−176.6 (2)	C3B—S1B—C1B—N1B	−0.1 (2)
C1A—N1A—C2A—C3A	0.2 (3)	C3B—S1B—C1B—C4	−179.6 (2)
Cu1^{ii}—N1A—C2A—C3A	−155.55 (18)	C1B—N1B—C2B—C3B	−0.5 (3)
C1A—N1A—C2A—C4A	177.6 (2)	Cu1—N1B—C2B—C3B	177.75 (17)
Cu1^{ii}—N1A—C2A—C4A	21.8 (2)	C1B—N1B—C2B—C4B	−178.3 (2)
N1A—C2A—C3A—S1A	0.3 (3)	Cu1—N1B—C2B—C4B	−0.1 (3)
C4A—C2A—C3A—S1A	−176.7 (2)	N1B—C2B—C3B—S1B	0.4 (3)
C1A—S1A—C3A—C2A	−0.6 (2)	C4B—C2B—C3B—S1B	178.0 (2)
C8A—N2A—C4A—C5A	2.3 (3)	C1B—S1B—C3B—C2B	−0.2 (2)
Cu1^{ii}—N2A—C4A—C5A	−170.47 (19)	C8B—N2B—C4B—C5B	−1.8 (4)
C8A—N2A—C4A—C2A	−178.9 (2)	Cu1—N2B—C4B—C5B	177.81 (19)
Cu1^{ii}—N2A—C4A—C2A	8.3 (3)	C8B—N2B—C4B—C2B	178.2 (2)
C3A—C2A—C4A—N2A	155.6 (2)	Cu1—N2B—C4B—C2B	−2.2 (3)
N1A—C2A—C4A—N2A	−21.4 (3)	C3B—C2B—C4B—N2B	−176.0 (2)
C3A—C2A—C4A—C5A	−25.6 (4)	N1B—C2B—C4B—N2B	1.5 (3)
N1A—C2A—C4A—C5A	157.4 (2)	C3B—C2B—C4B—C5B	4.0 (4)
N2A—C4A—C5A—C6A	−1.4 (4)	N1B—C2B—C4B—C5B	−178.5 (2)
C2A—C4A—C5A—C6A	179.9 (2)	N2B—C4B—C5B—C6B	2.3 (4)
C4A—C5A—C6A—C7A	−0.7 (4)	C2B—C4B—C5B—C6B	−177.7 (2)
C5A—C6A—C7A—C8A	1.8 (4)	C4B—C5B—C6B—C7B	−1.0 (4)
C4A—N2A—C8A—C7A	−1.1 (4)	C5B—C6B—C7B—C8B	−0.6 (4)
Cu1^{ii}—N2A—C8A—C7A	170.5 (2)	C4B—N2B—C8B—C7B	0.0 (4)
C6A—C7A—C8A—N2A	−1.0 (4)	Cu1—N2B—C8B—C7B	−179.53 (19)
N2A^{i}—Cu1—N1B—C1B	−35.2 (3)	C6B—C7B—C8B—N2B	1.2 (4)

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