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Crystal structure of aquabis(heptafluorobutanoato-κO)(1,10′-phenanthroline-$\kappa^2 N,N'$)copper(II)

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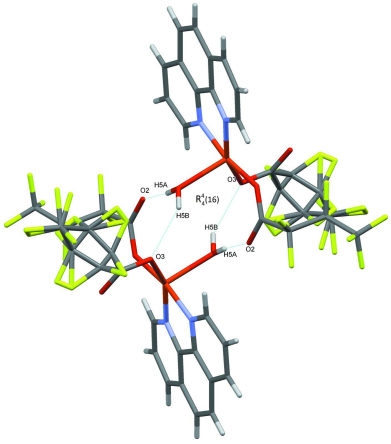
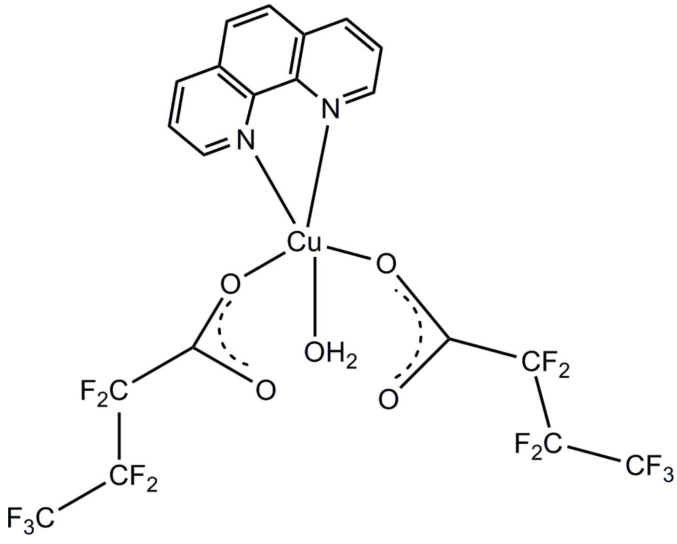
The title compound, $[Cu(C_4F_7O_2)_2(C_{12}H_8N_2)(H_2O)]$, is mononuclear and contains a pentacoordinated Cu^{II} ion. The geometry of Cu^{II} ion can be described as distorted square-pyramidal with two O atoms of two butanoate anions and two N atoms of the *o*-phenanthroline ligand occupying the basal plane, and a water O atom located at the axial position. In the crystal, C—H···(O,F) and O—H···(O,F) hydrogen bonds and π–π interactions [centroid-to-centroid distance 3.533 (2) Å] link the molecules into a three-dimensional supramolecular structure.

1. Chemical context

Over the past decades, vast efforts have been dedicated to the rational design and synthesis of metal-carboxylate coordination polymers due to their potential applications in medicine, electronics, magnetism, catalysis, gas storage, *etc* (Ahmad *et al.*, 2014; Patel *et al.*, 2013). In addition, metal–*o*-phenanthroline complexes and their derivatives have attracted much attention because of their unusual features (Ma *et al.*, 2004; Bi *et al.*, 2004; Wall *et al.*, 1999; Naing *et al.*, 1995). This work reports a new copper coordination complex, $[Cu(C_4F_7O_2)_2(C_{12}H_8N_2)(H_2O)]$, resulting from the reaction of heptafluorobutanoic acid and Cu^{II} ions in the presence of *o*-phenanthroline.





2. Structural commentary

The neutral complex $[Cu(C_4F_7O_2)_2(C_{12}H_8N_2)(H_2O)]$ is composed of a central Cu^{II} ion, coordinated by two oxygen atoms (O1 and O3) of two butanoate anions, an oxygen atom

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.942 (3)	Cu1—N1	2.019 (3)
Cu1—O3	1.980 (3)	Cu1—O5	2.173 (3)
Cu1—N2	2.007 (3)		
O1—Cu1—O3	96.11 (11)	N2—Cu1—N1	81.75 (12)
O1—Cu1—N2	169.16 (12)	O1—Cu1—O5	97.20 (12)
O3—Cu1—N2	90.37 (12)	O3—Cu1—O5	96.84 (12)
O1—Cu1—N1	88.94 (11)	N2—Cu1—O5	90.61 (12)
O3—Cu1—N1	156.71 (11)	N1—Cu1—O5	105.09 (12)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{i}	0.95	2.33	3.196 (5)	151
C6—H6···F4^{i}	0.95	2.54	3.217 (5)	128
O5—H5*B*···F10^{ii}	0.84 (2)	2.45 (6)	2.931 (6)	117 (5)
O5—H5*B*···O3^{ii}	0.84 (2)	2.31 (5)	2.881 (4)	125 (4)
O5—H5*A*···O2^{ii}	0.84 (2)	1.87 (2)	2.707 (5)	175 (6)
C1—H1···O1	0.95	2.49	2.974 (5)	111

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

(O5) of the water molecule, and two nitrogen atoms (N1 and N2) of the *N*,*N*′–chelating *o*–phenanthroline ligand (Fig. 1). Selected geometric parameters are presented in Table 1. The coordination about the Cu^{II} ion is better described as a square-pyramid. The geometry parameter τ, which is defined as $\tau = (\beta - \alpha)/60$, is applicable to five-coordinate structures within the structural continuum between trigonal–bipyramidal and tetragonal or rectangular pyramidal. For perfect tetragonal symmetry, τ is zero, and for perfect trigonal–bipyramidal geometry, τ becomes 1.0 (Addison *et al.*, 1984). In the title compound, the largest angles within the four atoms N1, N2, O2, O3 are β = 169.16 (12)° for O1–Cu1—N2, and α = 156.71 (11)° for N1—Cu1—O3. Thus, τ is 0.21, indicating a 79% rectangular pyramidal geometry.

The Cu—O bonds [1.942 (3) and 1.980 (3) Å] in the quadrilateral plane are shorter than the apical position [2.173 (3) Å]. The mean Cu—N(phen) distance of 2.043 Å and the bite angle N1—Cu1—N2 of 81.75 (12)° are close to the corresponding values observed in related copper–*o*-phenanthroline compounds (Beghidja *et al.*, 2014; Awaleh *et al.*, 2005). The cisoid bond angles are in the range 81.75 (12)–96.11 (11)°, and transoid ones are 156.71 (11)°, and 169.16 (12)° exhibiting substantial deviations from 90 and 180° for a square. These are consistent with literature values (Jing *et al.*, 2011). An intramolecular C1—H1···O1 hydrogen bond occurs.

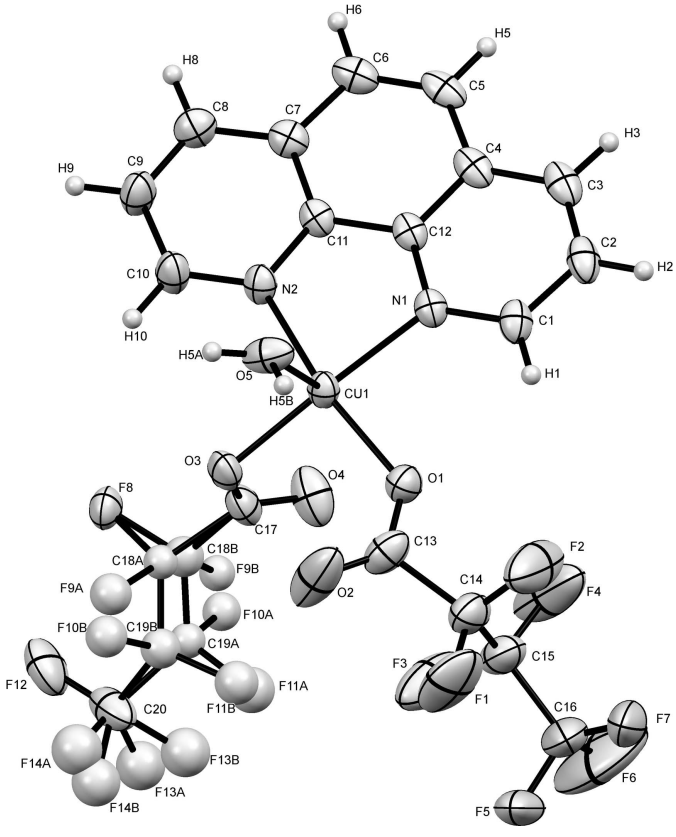


Figure 1
The molecular structure of title compound, with displacement ellipsoids shown at the 30% probability level.

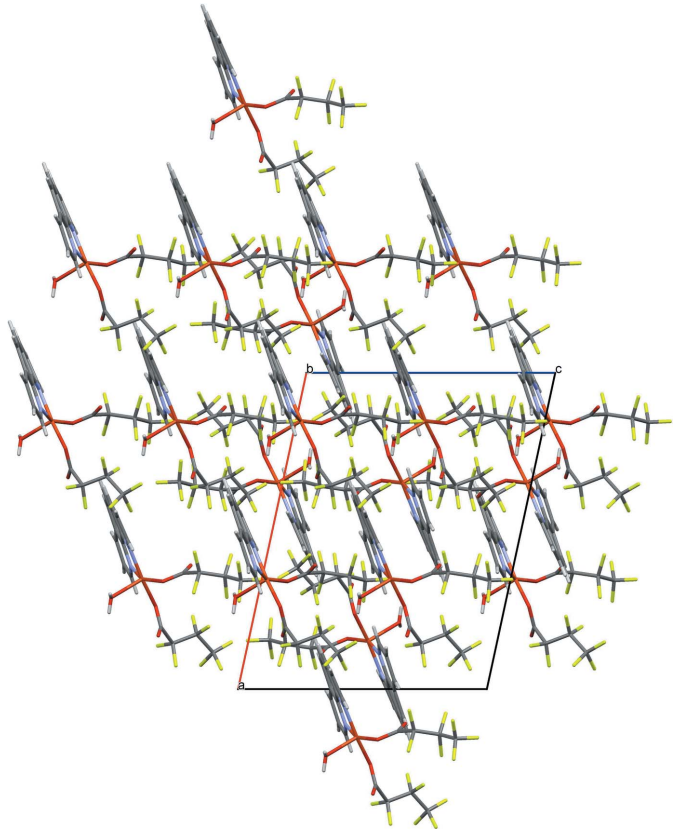


Figure 2
A partial view of the packing of the title complex, showing the formation of a hydrogen-bond pattern as well as edge-fused $R_4^4(16)$ rings. [Symmetry code: $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$.]

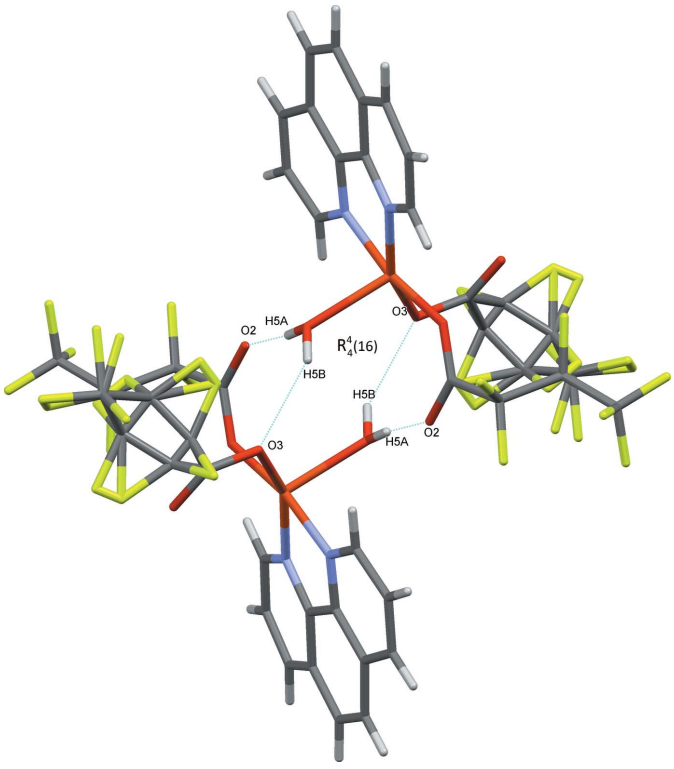


Figure 3
Representative O—H···O, C—H···O and C—H···F and π–π stacking interactions viewed along the *c* axis are drawn as dotted lines.

3. Supramolecular features

In the crystal, intermolecular O—H···O, C—H···O and C—H···F hydrogen bonds (Table 2) link the molecules into a three-dimensional network (Fig. 2). The oxygen atom (O5) of the water molecule acts as a hydrogen-bond donor, *via* atoms H5*A* and H5*B*, to oxygen atom O3 of one coordinating carboxylate group ($-x+\frac{1}{2}, -y+\frac{1}{2}, -z$) and to the dangling oxygen atom O2 of the other coordinating carboxylate group ($-x+\frac{1}{2}, -y+\frac{1}{2}, -z$), thus enclosing centrosymmetric $R_4^4(16)$ ring motifs (Bernstein *et al.*, 1995) running parallel to the *b*-axis direction (Fig. 3). In addition, C—H···F and O—H···F hydrogen bonds are formed, (C6—H6···F4 and O5—H5*B*···F10; Table 2; Fig. 3); the H···F distances are comparable with those reported for C—H···F interactions (2.44–2.90 Å; Dunitz & Taylor *et al.*, 1997, Bianchi *et al.*, 2003; Lee *et al.*, 2000).

In the crystal, the packing appears to be influenced by π–π stacking interactions between *o*-phenanthroline ring systems of neighboring molecules, with the distance between the centroids of the N1/C1–C4/C12 and C4–C7/C11/C12 rings being 3.533 (2) Å. (Fig. 4). The shortest Cu···Cu distance in the supramolecular structure is 7.845 Å.

4. Database survey

For heptafluorobutanoic acid, see: Sokolov *et al.* (2011); Awaleh *et al.* (2005); King *et al.* (2009). For related structures and *o*-phenanthroline, see: Beghidja *et al.* (2014); Awaleh *et al.* (2005); Huang *et al.* (2010); Liu *et al.* (2010); Jing *et al.* (2011); Ma *et al.* (2004); Ni *et al.* (2011); Meundaeng *et al.* (2013); Sokolov *et al.* (2011); Yin *et al.* (2011).

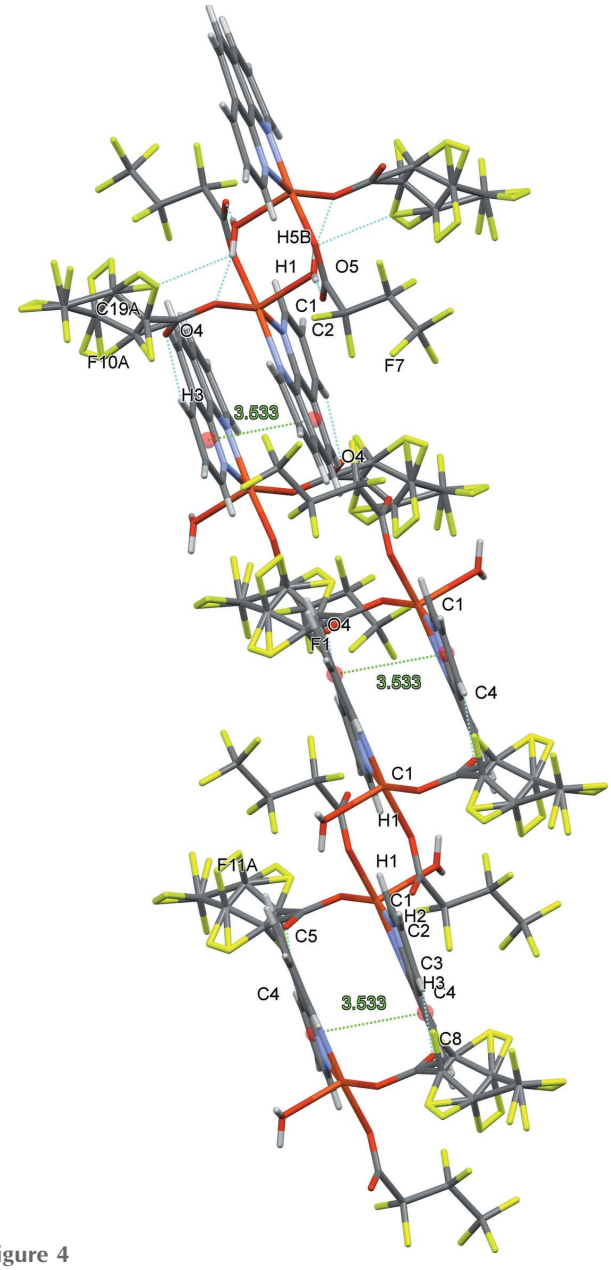


Figure 4
π–π interactions in the title compound.

5. Synthesis and crystallization

$Cu(ClO4)\cdot 6H_2O$ in methanol (0.076 mmol, 0.19 g) was added to a solution of *o*-phenanthroline (0.076 mmol, 0.14 g) and heptafluorobutanoic acid (0.0160 mmol, 0.1ml) in methanol (7 ml). Afterwards the obtained transparent blue solution was left to evaporate slowly in the air at ambient temperature and after two weeks, X-ray quality crystals appeared as blue plates. They were filtered off, washed with diethyl ether and dried in the air. Yield: 46 mg, 86%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were placed in calculated positions and refined as riding with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The coordinates of the water H atoms were refined, and U_{iso}(H) was set to be 2U_{eq}(O). One of the heptafluorobutanoate groups is disordered over two sets of sites in a 0.705 (9):0.955 (9) ratio. Atoms associated with the disorder were refined with isotropic displacement parameters.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_4F_7O_2)_2(C_{12}H_8N_2)(H_2O)]$
M_r	687.84
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	110
a, *b*, *c* (Å)	18.0213 (5), 19.4619 (6), 13.8664 (4)
β (°)	102.205 (1)
V (Å^3)	4753.4 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.07
Crystal size (mm)	0.35 × 0.26 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.707, 0.815
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22348, 5892, 4467
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.156, 0.95
No. of reflections	5892
No. of parameters	450
No. of restraints	21
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.59, −1.08

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012).

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supporting information

Acta Cryst. (2016). E**72**, 4-7 [doi:10.1107/S2056989015022720]

Crystal structure of aquabis(heptafluorobutanoato-κO)(1,10′-phenanthroline-$\kappa^2 N,N'$)copper(II)

Ibrahim Kani

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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: *WinGX* (Farrugia, 2012).

Aquabis(heptafluorobutanoato-κO)(1,10′-phenanthroline-$\kappa^2 N,N'$)copper(II)

Crystal data

$[Cu(C_4F_7O_2)_2(C_{12}H_8N_2)(H_2O)]$
M_r = 687.84
Monoclinic, $C2/c$
a = 18.0213 (5) Å
b = 19.4619 (6) Å
c = 13.8664 (4) Å
β = 102.205 (1)°
V = 4753.4 (2) Å^3
Z = 8
$F(000)$ = 2712
D_x = 1.922 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6696 reflections
θ = 2.3–27.3°
μ = 1.07 mm^{-1}
T = 110 K
Plate, green
0.35 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.707, T_{max} = 0.815
22348 measured reflections
5892 independent reflections
4467 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −22→24
k = −25→25
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.156
S = 0.95
5892 reflections
450 parameters
21 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 30.9575P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.59$ e Å^{-3}
$\Delta\rho_{min} = -1.08$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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)
C1	0.1436 (2)	−0.00631 (18)	−0.0275 (3)	0.0331 (8)	
H1	0.1945	−0.0102	0.0084	0.040*	
C2	0.1051 (3)	−0.06556 (19)	−0.0674 (3)	0.0384 (9)	
H2	0.1301	−0.1088	−0.0597	0.046*	
C3	0.0312 (2)	−0.06099 (19)	−0.1176 (3)	0.0363 (8)	
H3	0.0045	−0.1012	−0.1439	0.044*	
C4	−0.0050 (2)	0.00320 (18)	−0.1299 (3)	0.0314 (7)	
C5	−0.0812 (2)	0.0146 (2)	−0.1834 (3)	0.0350 (8)	
H5	−0.1121	−0.0237	−0.2083	0.042*	
C6	−0.1098 (2)	0.0786 (2)	−0.1991 (3)	0.0358 (8)	
H6	−0.1600	0.0846	−0.2364	0.043*	
C7	−0.0660 (2)	0.13790 (19)	−0.1606 (3)	0.0310 (7)	
C8	−0.0907 (2)	0.2063 (2)	−0.1761 (3)	0.0377 (8)	
H8	−0.1395	0.2161	−0.2153	0.045*	
C9	−0.0445 (2)	0.2586 (2)	−0.1347 (3)	0.0417 (9)	
H9	−0.0604	0.3049	−0.1460	0.050*	
C10	0.0269 (2)	0.24334 (19)	−0.0752 (3)	0.0378 (8)	
H10	0.0581	0.2800	−0.0450	0.045*	
C11	0.00687 (19)	0.12756 (17)	−0.1035 (2)	0.0265 (7)	
C12	0.03820 (19)	0.06005 (17)	−0.0895 (2)	0.0261 (7)	
C13	0.3038 (2)	0.1216 (2)	0.1361 (3)	0.0446 (10)	
C14	0.3553 (3)	0.0667 (2)	0.1973 (3)	0.0497 (11)	
C15	0.3264 (3)	0.0430 (3)	0.2862 (3)	0.0532 (12)	
C16	0.3843 (4)	0.0061 (3)	0.3681 (4)	0.0755 (18)	
C17	0.1326 (2)	0.21520 (19)	0.1794 (3)	0.0378 (8)	
Cu1	0.15206 (2)	0.14635 (2)	0.01889 (3)	0.02752 (13)	
F1	0.42548 (17)	0.0915 (2)	0.2295 (3)	0.0965 (13)	
F2	0.3629 (3)	0.0143 (2)	0.1396 (3)	0.122 (2)	
F3	0.3026 (2)	0.0984 (2)	0.3269 (2)	0.1035 (16)	
F4	0.2709 (2)	−0.0012 (3)	0.2555 (4)	0.146 (3)	
F5	0.4354 (2)	0.04972 (17)	0.4146 (2)	0.0900 (13)	
F6	0.3516 (3)	−0.0217 (4)	0.4308 (4)	0.187 (3)	

F7	0.4236 (3)	−0.03979 (16)	0.3298 (3)	0.1140 (18)	
N1	0.11117 (17)	0.05511 (14)	−0.0382 (2)	0.0272 (6)	
N2	0.05191 (16)	0.17936 (15)	−0.0599 (2)	0.0296 (6)	
O1	0.23861 (16)	0.09849 (14)	0.09756 (19)	0.0376 (6)	
O2	0.33070 (19)	0.1784 (2)	0.1330 (4)	0.0850 (15)	
O3	0.15945 (15)	0.22857 (13)	0.1045 (2)	0.0358 (6)	
O4	0.1086 (2)	0.16038 (16)	0.2021 (3)	0.0548 (9)	
O5	0.21033 (16)	0.18964 (17)	−0.0891 (2)	0.0435 (7)	
C19A	0.1413 (3)	0.2694 (3)	0.3503 (4)	0.0340 (14)	0.705 (9)
C18A	0.1341 (3)	0.2831 (3)	0.2401 (4)	0.0308 (14)	0.705 (9)
F10	0.1905 (3)	0.3264 (2)	0.2301 (4)	0.0468 (12)	0.705 (9)
F10A	0.0794 (3)	0.2369 (3)	0.3662 (4)	0.0391 (11)	0.705 (9)
F11A	0.2022 (3)	0.2288 (2)	0.3824 (4)	0.0542 (13)	0.705 (9)
F13A	0.1512 (3)	0.3159 (3)	0.5086 (4)	0.0653 (15)	0.705 (9)
F14A	0.2185 (6)	0.3659 (6)	0.4174 (5)	0.067 (2)	0.705 (9)
C18B	0.1086 (7)	0.2638 (6)	0.2581 (8)	0.031 (3)	0.295 (9)
C19B	0.1812 (6)	0.2937 (6)	0.3221 (8)	0.033 (3)	0.295 (9)
F9B	0.0682 (7)	0.2367 (6)	0.3213 (9)	0.034 (2)	0.295 (9)
F10B	0.2100 (7)	0.3414 (6)	0.2688 (9)	0.040 (2)	0.295 (9)
F11B	0.2321 (6)	0.2427 (5)	0.3454 (9)	0.046 (3)	0.295 (9)
F13B	0.1619 (7)	0.2812 (7)	0.4850 (8)	0.055 (3)	0.295 (9)
F14B	0.2290 (11)	0.3614 (15)	0.4558 (11)	0.063 (5)	0.295 (9)
F8	0.06788 (13)	0.31602 (11)	0.20682 (16)	0.0373 (5)	
F12	0.10008 (19)	0.37634 (14)	0.3905 (2)	0.0641 (8)	
C20	0.1565 (3)	0.3330 (2)	0.4172 (3)	0.0571 (13)	
H5A	0.200 (3)	0.2313 (13)	−0.100 (5)	0.086*	
H5B	0.2577 (13)	0.185 (3)	−0.081 (5)	0.086*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.043 (2)	0.0282 (17)	0.0332 (18)	0.0037 (15)	0.0187 (16)	0.0015 (14)
C2	0.060 (3)	0.0249 (17)	0.0364 (19)	0.0036 (16)	0.0247 (18)	−0.0016 (14)
C3	0.054 (2)	0.0292 (17)	0.0328 (18)	−0.0083 (16)	0.0249 (17)	−0.0060 (14)
C4	0.0391 (19)	0.0321 (17)	0.0289 (16)	−0.0094 (15)	0.0207 (15)	−0.0066 (14)
C5	0.039 (2)	0.042 (2)	0.0291 (17)	−0.0145 (16)	0.0179 (15)	−0.0131 (15)
C6	0.0314 (19)	0.049 (2)	0.0299 (17)	−0.0093 (16)	0.0124 (15)	−0.0076 (16)
C7	0.0293 (17)	0.0372 (19)	0.0297 (16)	−0.0024 (14)	0.0130 (14)	−0.0025 (14)
C8	0.0292 (18)	0.044 (2)	0.040 (2)	0.0023 (16)	0.0086 (15)	0.0013 (17)
C9	0.033 (2)	0.0312 (19)	0.059 (3)	0.0060 (15)	0.0050 (18)	0.0054 (18)
C10	0.0318 (19)	0.0266 (17)	0.054 (2)	−0.0013 (14)	0.0066 (17)	0.0010 (16)
C11	0.0274 (16)	0.0270 (15)	0.0287 (16)	−0.0049 (13)	0.0144 (13)	−0.0016 (13)
C12	0.0294 (17)	0.0266 (15)	0.0269 (15)	−0.0031 (13)	0.0165 (13)	−0.0029 (12)
C13	0.033 (2)	0.056 (3)	0.045 (2)	0.0097 (19)	0.0077 (17)	0.0139 (19)
C14	0.053 (3)	0.047 (2)	0.044 (2)	0.015 (2)	−0.0026 (19)	−0.0041 (19)
C15	0.049 (3)	0.052 (3)	0.049 (2)	−0.009 (2)	−0.012 (2)	0.015 (2)
C16	0.100 (5)	0.056 (3)	0.053 (3)	0.005 (3)	−0.025 (3)	0.008 (3)
C17	0.037 (2)	0.0278 (18)	0.048 (2)	−0.0001 (15)	0.0085 (17)	−0.0129 (16)

Cu1	0.0256 (2)	0.0237 (2)	0.0338 (2)	−0.00175 (16)	0.00763 (16)	0.00126 (16)
F1	0.0325 (15)	0.120 (3)	0.128 (3)	0.0171 (17)	−0.0034 (17)	0.051 (3)
F2	0.175 (4)	0.108 (3)	0.061 (2)	0.099 (3)	−0.027 (2)	−0.033 (2)
F3	0.115 (3)	0.151 (4)	0.0462 (17)	0.081 (3)	0.0195 (18)	0.009 (2)
F4	0.094 (3)	0.141 (4)	0.162 (4)	−0.081 (3)	−0.066 (3)	0.109 (3)
F5	0.110 (3)	0.065 (2)	0.0649 (19)	0.0228 (19)	−0.0494 (19)	−0.0231 (16)
F6	0.147 (5)	0.268 (8)	0.127 (4)	−0.009 (5)	−0.010 (4)	0.148 (5)
F7	0.171 (4)	0.0399 (17)	0.090 (3)	0.039 (2)	−0.064 (3)	−0.0144 (17)
N1	0.0322 (15)	0.0250 (13)	0.0279 (13)	−0.0003 (11)	0.0146 (12)	−0.0006 (11)
N2	0.0248 (14)	0.0259 (14)	0.0395 (16)	−0.0015 (11)	0.0097 (12)	0.0022 (12)
O1	0.0396 (15)	0.0344 (14)	0.0362 (13)	0.0061 (11)	0.0022 (11)	−0.0013 (11)
O2	0.0348 (18)	0.077 (3)	0.131 (4)	−0.0168 (17)	−0.010 (2)	0.060 (3)
O3	0.0354 (14)	0.0245 (12)	0.0457 (15)	−0.0064 (10)	0.0045 (12)	−0.0028 (11)
O4	0.064 (2)	0.0404 (16)	0.071 (2)	−0.0094 (15)	0.0411 (18)	−0.0060 (15)
O5	0.0326 (14)	0.0626 (19)	0.0336 (14)	−0.0162 (13)	0.0033 (12)	0.0108 (13)
C19A	0.036 (3)	0.022 (2)	0.043 (3)	−0.003 (2)	0.009 (2)	0.001 (2)
C18A	0.034 (3)	0.017 (2)	0.046 (3)	−0.007 (2)	0.017 (2)	−0.006 (2)
F10	0.060 (3)	0.031 (2)	0.060 (3)	−0.0265 (18)	0.036 (3)	−0.019 (2)
F10A	0.049 (3)	0.0278 (17)	0.046 (3)	−0.0078 (16)	0.022 (2)	0.004 (2)
F11A	0.046 (3)	0.044 (2)	0.068 (3)	0.0102 (19)	0.001 (2)	0.006 (2)
F13A	0.099 (4)	0.059 (3)	0.035 (2)	−0.008 (3)	0.007 (2)	−0.003 (2)
F14A	0.080 (4)	0.063 (4)	0.062 (5)	−0.034 (3)	0.020 (4)	−0.017 (5)
C18B	0.030 (7)	0.025 (7)	0.038 (7)	−0.002 (5)	0.007 (6)	0.005 (5)
C19B	0.039 (7)	0.032 (6)	0.027 (6)	−0.004 (5)	0.006 (5)	0.002 (5)
F9B	0.034 (5)	0.031 (4)	0.040 (6)	−0.006 (3)	0.015 (5)	0.002 (5)
F10B	0.052 (6)	0.031 (5)	0.045 (6)	−0.017 (4)	0.024 (5)	−0.007 (4)
F11B	0.032 (5)	0.045 (5)	0.055 (6)	0.006 (4)	−0.004 (4)	−0.006 (4)
F13B	0.065 (7)	0.072 (8)	0.028 (5)	−0.028 (6)	0.007 (4)	0.003 (5)
F14B	0.087 (12)	0.063 (8)	0.054 (10)	−0.021 (8)	0.046 (9)	−0.013 (10)
F8	0.0431 (13)	0.0271 (10)	0.0419 (12)	0.0077 (9)	0.0096 (10)	0.0026 (9)
F12	0.092 (2)	0.0404 (14)	0.0661 (18)	−0.0051 (15)	0.0298 (17)	−0.0202 (13)
C20	0.091 (4)	0.046 (2)	0.033 (2)	−0.024 (3)	0.010 (2)	−0.0066 (18)

Geometric parameters (Å, º)

C1—N1	1.325 (4)	C15—C16	1.546 (7)
C1—C2	1.398 (5)	C16—F6	1.271 (8)
C1—H1	0.9500	C16—F5	1.316 (7)
C2—C3	1.369 (6)	C16—F7	1.319 (8)
C2—H2	0.9500	C17—O4	1.218 (5)
C3—C4	1.403 (5)	C17—O3	1.261 (5)
C3—H3	0.9500	C17—C18A	1.564 (6)
C4—C12	1.400 (5)	C17—C18B	1.572 (11)
C4—C5	1.433 (6)	Cu1—O1	1.942 (3)
C5—C6	1.348 (6)	Cu1—O3	1.980 (3)
C5—H5	0.9500	Cu1—N2	2.007 (3)
C6—C7	1.437 (5)	Cu1—N1	2.019 (3)
C6—H6	0.9500	Cu1—O5	2.173 (3)

C7—C11	1.397 (5)	O5—H5A	0.840 (19)
C7—C8	1.406 (5)	O5—H5B	0.843 (19)
C8—C9	1.362 (6)	C19A—F10A	1.341 (7)
C8—H8	0.9500	C19A—F11A	1.349 (6)
C9—C10	1.405 (5)	C19A—C18A	1.530 (7)
C9—H9	0.9500	C19A—C20	1.536 (7)
C10—N2	1.326 (5)	C18A—F8	1.348 (6)
C10—H10	0.9500	C18A—F10	1.349 (8)
C11—N2	1.354 (4)	F13A—C20	1.332 (6)
C11—C12	1.427 (5)	F14A—C20	1.288 (9)
C12—N1	1.360 (4)	C18B—F9B	1.359 (15)
C13—O2	1.211 (6)	C18B—F8	1.363 (11)
C13—O1	1.265 (5)	C18B—C19B	1.532 (12)
C13—C14	1.546 (6)	C19B—F11B	1.344 (12)
C14—F2	1.321 (5)	C19B—F10B	1.357 (13)
C14—F1	1.339 (6)	C19B—C20	1.665 (13)
C14—C15	1.508 (7)	F13B—C20	1.366 (11)
C15—F4	1.321 (6)	F14B—C20	1.417 (16)
C15—F3	1.329 (6)	F12—C20	1.313 (6)

N1—C1—C2	122.0 (4)	O3—Cu1—N2	90.37 (12)
N1—C1—H1	119.0	O1—Cu1—N1	88.94 (11)
C2—C1—H1	119.0	O3—Cu1—N1	156.71 (11)
C3—C2—C1	119.7 (4)	N2—Cu1—N1	81.75 (12)
C3—C2—H2	120.1	O1—Cu1—O5	97.20 (12)
C1—C2—H2	120.1	O3—Cu1—O5	96.84 (12)
C2—C3—C4	119.8 (3)	N2—Cu1—O5	90.61 (12)
C2—C3—H3	120.1	N1—Cu1—O5	105.09 (12)
C4—C3—H3	120.1	C1—N1—C12	118.5 (3)
C12—C4—C3	116.7 (3)	C1—N1—Cu1	129.3 (3)
C12—C4—C5	118.4 (3)	C12—N1—Cu1	112.0 (2)
C3—C4—C5	124.8 (3)	C10—N2—C11	118.4 (3)
C6—C5—C4	121.2 (3)	C10—N2—Cu1	128.6 (3)
C6—C5—H5	119.4	C11—N2—Cu1	113.0 (2)
C4—C5—H5	119.4	C13—O1—Cu1	129.1 (3)
C5—C6—C7	121.4 (4)	C17—O3—Cu1	109.7 (2)
C5—C6—H6	119.3	Cu1—O5—H5A	112 (4)
C7—C6—H6	119.3	Cu1—O5—H5B	120 (4)
C11—C7—C8	116.9 (3)	H5A—O5—H5B	108 (3)
C11—C7—C6	118.2 (3)	F10A—C19A—F11A	108.4 (5)
C8—C7—C6	124.9 (4)	F10A—C19A—C18A	110.4 (5)
C9—C8—C7	119.8 (4)	F11A—C19A—C18A	108.8 (5)
C9—C8—H8	120.1	F10A—C19A—C20	109.2 (5)
C7—C8—H8	120.1	F11A—C19A—C20	104.1 (4)
C8—C9—C10	119.5 (4)	C18A—C19A—C20	115.5 (4)
C8—C9—H9	120.2	F8—C18A—F10	107.4 (5)
C10—C9—H9	120.2	F8—C18A—C19A	107.8 (4)
N2—C10—C9	122.0 (4)	F10—C18A—C19A	107.7 (5)

N2—C10—H10	119.0	F8—C18A—C17	107.7 (4)
C9—C10—H10	119.0	F10—C18A—C17	113.6 (4)
N2—C11—C7	123.3 (3)	C19A—C18A—C17	112.3 (4)
N2—C11—C12	116.2 (3)	F9B—C18B—F8	108.9 (9)
C7—C11—C12	120.5 (3)	F9B—C18B—C19B	106.3 (10)
N1—C12—C4	123.3 (3)	F8—C18B—C19B	108.5 (9)
N1—C12—C11	116.6 (3)	F9B—C18B—C17	118.6 (9)
C4—C12—C11	120.1 (3)	F8—C18B—C17	106.5 (7)
O2—C13—O1	130.7 (4)	C19B—C18B—C17	107.7 (9)
O2—C13—C14	116.8 (4)	F11B—C19B—F10B	108.4 (11)
O1—C13—C14	112.5 (4)	F11B—C19B—C18B	108.3 (9)
F2—C14—F1	105.6 (5)	F10B—C19B—C18B	108.8 (11)
F2—C14—C15	110.9 (5)	F11B—C19B—C20	115.6 (9)
F1—C14—C15	107.6 (4)	F10B—C19B—C20	108.4 (9)
F2—C14—C13	109.1 (4)	C18B—C19B—C20	107.2 (8)
F1—C14—C13	110.4 (4)	C18A—F8—C18B	29.1 (5)
C15—C14—C13	112.9 (4)	F14A—C20—F12	107.5 (7)
F4—C15—F3	112.0 (5)	F14A—C20—F13A	111.0 (5)
F4—C15—C14	107.7 (4)	F12—C20—F13A	102.8 (5)
F3—C15—C14	107.3 (4)	F14A—C20—F13B	115.4 (8)
F4—C15—C16	106.4 (4)	F12—C20—F13B	127.3 (7)
F3—C15—C16	107.1 (4)	F13A—C20—F13B	34.1 (5)
C14—C15—C16	116.5 (5)	F14A—C20—F14B	22.1 (8)
F6—C16—F5	108.4 (6)	F12—C20—F14B	116.9 (13)
F6—C16—F7	110.6 (6)	F13A—C20—F14B	89.1 (8)
F5—C16—F7	104.8 (6)	F13B—C20—F14B	95.9 (11)
F6—C16—C15	111.3 (6)	F14A—C20—C19A	116.4 (6)
F5—C16—C15	110.7 (4)	F12—C20—C19A	108.6 (4)
F7—C16—C15	110.8 (5)	F13A—C20—C19A	109.6 (4)
O4—C17—O3	127.8 (3)	F13B—C20—C19A	78.5 (7)
O4—C17—C18A	124.6 (4)	F14B—C20—C19A	125.1 (12)
O3—C17—C18A	107.6 (4)	F14A—C20—C19B	81.5 (6)
O4—C17—C18B	100.5 (5)	F12—C20—C19B	113.1 (5)
O3—C17—C18B	131.1 (5)	F13A—C20—C19B	136.4 (6)
C18A—C17—C18B	25.1 (4)	F13B—C20—C19B	102.4 (8)
O1—Cu1—O3	96.11 (11)	F14B—C20—C19B	95.6 (10)
O1—Cu1—N2	169.16 (12)	C19A—C20—C19B	36.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{i}	0.95	2.33	3.196 (5)	151
C6—H6···F4^{i}	0.95	2.54	3.217 (5)	128
O5—H5*B*···F10^{ii}	0.84 (2)	2.45 (6)	2.931 (6)	117 (5)
O5—H5*B*···O3^{ii}	0.84 (2)	2.31 (5)	2.881 (4)	125 (4)

O5—H5*A*···O2^{ii}	0.84 (2)	1.87 (2)	2.707 (5)	175 (6)
C1—H1···O1	0.95	2.49	2.974 (5)	111

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