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catena-Poly[2-amino-3-chloro-5-(trifluoromethyl)-pyridinium [[chloridocuprate]-di-μ-chlorido]]

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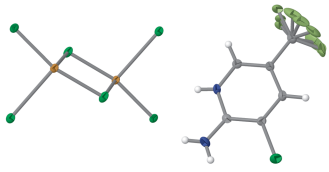
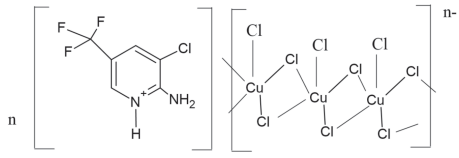
The reaction of 2-amino-3-chloro-5-trifluoromethylpyridine with copper(II) chloride dihydrate in aqueous HCl generated the title compound, $\{(C_6H_5ClF_3N_2)[CuCl_3]\}_n$. The structure comprises discrete cations and bichloride bridged chains of Cu^{II} ions with an additional terminal chloride ion attached to each Cu^{2+} ion. The Cu(II) ions are coordinated to five chloride ions (four bridging) in the form of a slightly distorted square pyramid with the terminal chloride ion in an equatorial site. The resulting chains run parallel to the crystallographic *b*-axis direction. The structure features N—H···Cl hydrogen bonds between the pyridinium and amino N—H donors and chlorido ions, and halogen bonds between the chlorido ions and fluorine atoms. The fluorine atoms of the trifluoromethyl group were refined as a three-fold disordered model.

3D view



Chemical scheme



Structure description

Five-coordinate, bi-bridged chloridocuprate chains have been prepared with a wide variety of ancillary organic cations. Perhaps the first such structure reported is *catena*-dimethylammonium trichloridocuprate (Willett, 1966). Since that time, a similar structure was been reported with 4-benzylpiperidinium (Battaglia *et al.*, 1980). Similar structures have been observed with chloride bridged chains, but where more than one coordination geometry is exhibited in the chain. The diethyldimethylammonium chloridocuprate salt (Fujii *et al.*, 1995) comprises a repeating chain of Cu^{II} ions *via* three bichloride bridges followed by a trichloride bridge with four crystallographically unique Cu ions. The ethyltrimethylammonium compound (Bond *et al.*, 1990) exhibits both octahedral and square-pyramidal chloridocuprate geometries with three bichloride bridges followed by two trichloride bridges. The tetramethylammonium complex crystallizes as a chain of

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Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.2418 (4)	Cu1—Cl2	2.3141 (4)
Cu1—Cl2^{i}	2.2868 (4)	Cu1—Cl3	2.7553 (4)
Cu1—Cl3^{ii}	2.2886 (4)		
Cl1—Cu1—Cl2^{i}	165.097 (17)	Cl1—Cu1—Cl3	94.459 (14)
Cl1—Cu1—Cl3^{ii}	93.655 (14)	Cl2^{i}—Cu1—Cl3	99.461 (14)
Cl2^{i}—Cu1—Cl3^{ii}	91.679 (15)	Cl3^{ii}—Cu1—Cl3	89.878 (14)
Cl1—Cu1—Cl2	89.738 (14)	Cl2—Cu1—Cl3	97.164 (15)
Cl2^{i}—Cu1—Cl2	83.303 (15)	Cu1^{i}—Cl2—Cu1	96.698 (15)
Cl3^{ii}—Cu1—Cl2	171.929 (17)	Cu1^{ii}—Cl3—Cu1	90.121 (14)

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

trichloride bridged six-coordinate Cu^{II} ions (Weenk & Spek, 1976) and the tetramethylarsenium salt crystallizes as square-pyramidal chlorocuprate ions bridged by both monochloride and bichloride bridges into a two-dimensional layer (Murray & Willett, 1993).

We have been studying the copper(II) halide salts of various substituted 2-aminopyridinium ions (Bellesis *et al.*, 2024; Bedford *et al.*, 2023; Huynh *et al.*, 2023) including salts and complexes of 5-trifluoromethyl-2-aminopyridine (Gale *et al.*, 2013; Forman *et al.*, 2014, 2015). Neutral complexes of the closely related 3-chloro-5-trifluoromethyl-2-aminopyridine (TFCAP) (Salah *et al.*, 2025; Chakraborty *et al.*, 2024) as well as the bichloride bridged cadmium chain salt (Karâa *et al.*, 2023) and the neutral compound itself (Tan *et al.*, 2008) are also known. In the course of our investigation of salts of this aminopyridine (Wikaira *et al.*, 2010) we serendipitously prepared the title compound, $\{[C_6H_5ClF_3N_2][CuCl_3]\}_n$ (**I**), and herein report its preparation and structure.

The asymmetric unit of (**I**) and copper coordination sphere are shown in Fig. 1. Selected bond lengths and angles are given in Table 1. The Cu^{II} ion is coordinated by five chloride ions (three independent) in a slightly distorted square pyramidal geometry ($\tau = 0.11$; Addison *et al.*, 1984) with Cl3 in the apical position. The equatorial chloride ions are roughly co-planar (mean deviation of constituent atoms = 0.065 Å) with the copper ion lying 0.202 (1) Å above that plane. As is typical,

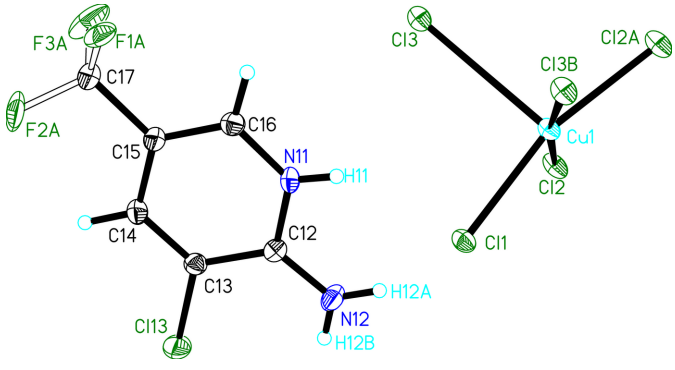

Figure 1
The asymmetric unit and copper coordination sphere of (**I**) shown as 50% probability ellipsoids. Hydrogen atoms are show as spheres of arbitrary size. The copper coordination sphere and those hydrogen atoms whose positions were refined are labeled. Only the major component of the three disordered positions for the CF_3 group is shown. Symmetry operations: (A) $-x, 2-y, -z$; (B) $-x, 1-y, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···Cl1	0.80 (2)	2.54 (2)	3.2496 (15)	148.6 (18)
N12—H12A···Cl1	0.85 (2)	2.53 (2)	3.2550 (17)	142.9 (17)
N12—H12B···Cl3^{iii}	0.79 (2)	2.62 (2)	3.3942 (15)	165 (2)

Symmetry code: (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

the axial Cu—Cl bond is lengthened by ∼0.5 Å relative to the equatorial Cu—Cl bonds.

As expected, the pyridine ring of the TFCAPH cation is virtually planar (mean deviation of constituent atoms = 0.006 Å) with N12 and Cl13 only slightly deviating from that plane (∼0.01Å). The –CF_3 substituent is significantly disordered and was refined using a three-site model to yield final occupancies of 0.346 (3):0.501 (3):0.153 (3) (see Fig. 2). The structure of TFCAP itself exhibits twofold disorder of the CF_3 group (Tan *et al.*, 2008) as do the salt $(TFCAPH)_2CuCl_4$ (Wikaira *et al.*, 2010) and the neutral $(TFCAP)_2CuCl_2$ complex (Salah *et al.*, 2025]. The C12—N11 and C16—N11 bond lengths are ∼0.18 Å longer in (**I**) than in TFCAP while the C12—N12 bond is comparably shorter. Other bond lengths within the ring differ by < 0.01 Å. Bond lengths within the ring are within 0.1 Å of those observed in the TFCAPH cations seen in the $(TFCAPH)_2CuX_4$ salts (X = Cl, Br) (Wikaira *et al.*, 2010). The greatest difference in angles within the ring is the C—N—C angle, 124.4 (1)° in **1** and 123–125° in the other pyridinium compounds, but only 118.4 (1)° in the free ligand (Tan *et al.*, 2008) and 118.8 (1)° in the neutral copper chlorido complex (Salah *et al.*, 2025).

The Cu^{II} ions are connected into a chain propagating parallel to the *b* axis *via* bibridged chloride linkages (Fig. 3).

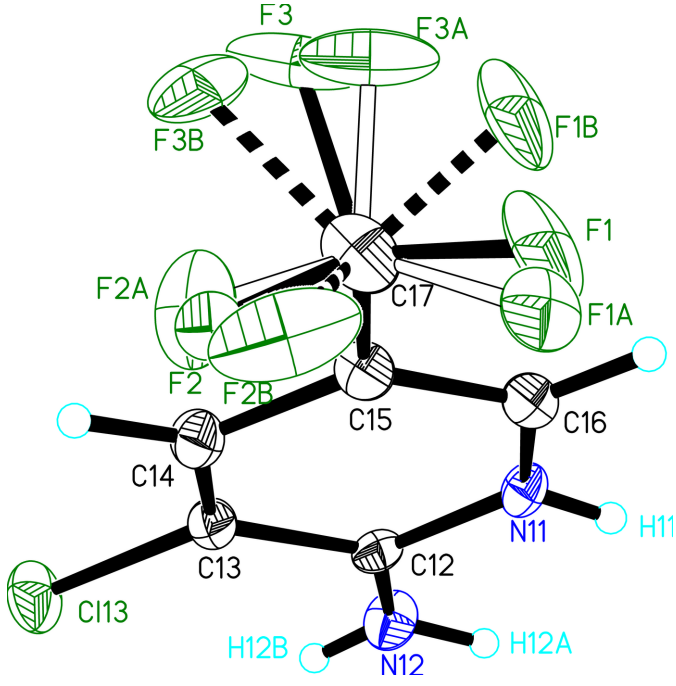

Figure 2
The threefold disordered CF_3 group of (**I**).

Table 3
Short interchain Cl···Cl contacts (Å, °).

d	angle	angle	τ	Symm. op.
Cl1···Cl1^{D} 3.92144 (4)	Cu1—Cl1···Cl1^{D} 107.886 (11)	Cl1···Cl1^{D}—Cu1^{D} 140.91 (5)	Cu1—Cl1···Cl1^{D}—Cu1^{D} −168.84 (1)	D: $-x, y-\frac{1}{2}, \frac{3}{2}-z$
Cl1···Cl2^{A} 3.8175 (5)	Cu1—Cl1···Cl2^{A} 169.888 (16)	Cl1···Cl2^{A}—Cu1^{F} 109.423 (14)	Cu1—Cl1···Cl2^{A}—Cu1^{F} 175.51 (1)	A: $x, \frac{3}{2}-y, z+\frac{1}{2}$; F: $-x, y+\frac{1}{2}, \frac{3}{2}-z$

The position of the terminal chloride ion (Cl1) alternates up and down relative to the *ab* plane as one passes along the chain. The bridges, Cl2/Cl2*A* and Cl3/Cl3*B*, form an alternating chain (Fig. 3). It is interesting to note that while the Cl2/Cl2*A* chloride ions bridge equatorial positions on adjacent copper ions, the Cl3/Cl3*A* bridges bridge axial/equatorial. The TFCAPH ions are linked to neighboring species by both hydrogen bonds (see Table 2) and halogen bonds (Fig. 4). Hydrogen bonds are observed between both the pyridinium and amino N—H donors and the terminal chlorido ions, and between the amino N—H donors and Cl3 within the chains (Table 2).

Type I halogen bonds (Cavallo *et al.*, 2016) are observed between Cl13 (on the pyridone ring) and fluorine atoms on the CF_3 group [Cl13···F1^{i} = 3.043 (11) Å, C13—Cl13···F1^{i} = 167.0 (3)°, Cl13···F1^{i}—C17^{i} = 139.4 (8); symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$] (see Fig. 4). Multiple short Cl···Cl contacts exist between chains, but only two are symmetry unique (see Table 3). Each Cl1 ion is close to two symmetry-equivalent Cl1 ions in neighboring chains and each Cl1 ion is close to one symmetry-equivalent Cl2 ion in a neighboring chain. These effectively link the chains into a sheet parallel to the *bc* plane. Such contacts have been shown to propagate magnetic exchange in CuX_4^{2-} complexes (Turnbull *et al.*, 2005).

Synthesis and crystallization

5-Trifluoromethyl-3-chloro-2-aminopyridine (TFCAP) and hydrochloric acid were purchased from the Aldrich Chemical Company and used without purification. Copper(II) chloride was obtained from J. T. Baker and used without purification. The IR spectrum was recorded on a Perkin-Elmer Spectrum 100 IR spectrophotometer; *s* = strong and *m* = medium. Combustion analyses were performed by the Marine Science Institute, U. California, Santa Barbara.

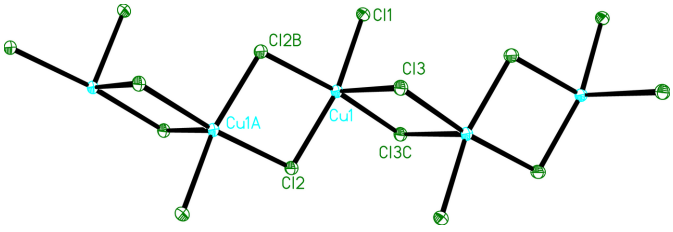

Figure 3
The chain structure of the $CuCl_3^-$ units in (**I**) shown as 50% probability ellipsoids viewed parallel to the *a*-axis direction (*b* horizontal). Symmetry operations: (A) $-x, 1-y, 1-z$; (B) $-x, 1-y, 1-z$; (C) $-x, 2-y, 1-z$.

TFCAP (0.394 g, 2.00 mmol) was dissolved in 2 ml of water and 1 ml of concentrated hydrochloric acid. Copper(II) chloride dihydrate (0.171 g, 1.00 mmol) was added and dissolved resulting in a bright green solution which was left at room temperature for slow evaporation. After three days, 0.382 g of green crystals of $(TFCAPH)_2CuCl_4$ (Wikaira *et al.*, 2010) were removed by filtration and the filtrate left for further evaporation. After two more weeks, brown crystals (purple when viewed individually under a microscope) were harvested by filtration [0.011 g, 8% correcting for recovered $(TFCAPH)_2CuCl_4$]. Elemental analysis (%) calculated for $C_6H_5Cl_4CuF_3N_2$, found (calculated): C 19.34 (19.61); H 1.49 (1.37); N 7.38 (7.62). IR, ν 3326*m*, 3198*m*, 3158*m*, 3113*m*, 3067*m*, 1661*s*, 1630*s*, 1325*s*, 1278*s*, 1178*m*, 1135*m*, 1100*m*, 1076*m*, 900*m*, 632*m* cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The fluorine atoms on the trifluoromethyl group were refined as a threefold disordered structure using both angle and distance restraints. Final occupancies for the three sets of fluorine atoms were 0.346 (3):0.501 (3):0.153 (3).

Acknowledgements

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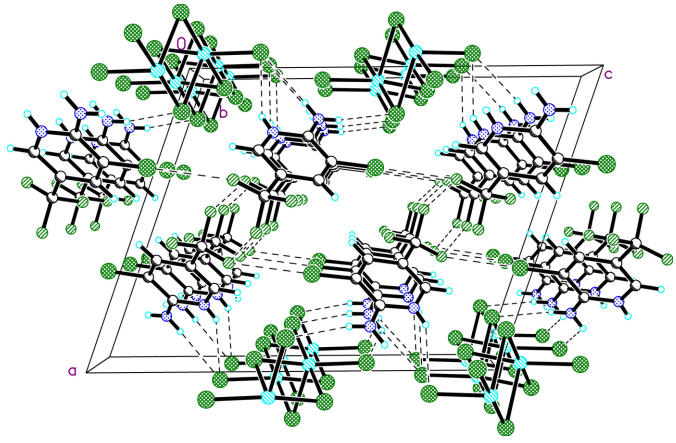

Figure 4
The unit-cell packing of (**I**) viewed parallel to the *b*-axis direction (the chain axis) with *c* horizontal. Dashed lines represent hydrogen bonds and halogen bonds. Only the major component of the disordered CF_3 group is shown.

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Funding information

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Table 4
Experimental details.

Crystal data	
Chemical formula	$(C_6H_5ClF_3N_2)[CuCl_3]$
M_r	367.46
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	110
a, b, c (Å)	12.2625 (4), 6.25540 (14), 15.7442 (4)
β (°)	109.341 (3)
V (Å^3)	1139.53 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.86
Crystal size (mm)	0.40 × 0.30 × 0.05
Data collection	
Diffractometer	Xcalibur, Ruby, Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.477, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9524, 3852, 3080
R_{int}	0.027
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.762
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.026, 0.059, 0.96
No. of reflections	3852
No. of parameters	211
No. of restraints	140
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.57

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *SHELXS2014* (Sheldrick, 2008), *SHELXL2019/2* (Sheldrick, 2015) and *XP* (Bruker, 1998).

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full crystallographic data

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Crystal data

$(C_6H_5ClF_3N_2)[CuCl_3]$
M_r = 367.46
Monoclinic, $P2_1/c$
a = 12.2625 (4) Å
b = 6.25540 (14) Å
c = 15.7442 (4) Å
β = 109.341 (3)°
V = 1139.53 (6) Å^3
Z = 4
$F(000)$ = 716
D_x = 2.142 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5156 reflections
θ = 5.1–32.7°
μ = 2.86 mm^{-1}
T = 110 K
Chip, purple
0.40 × 0.30 × 0.05 mm

Data collection

Xcalibur, Ruby, Gemini diffractometer
ω scans
Absorption correction: multi-scan (CrysAlisPro; Oxford Diffraction, 2009)
T_{min} = 0.477, T_{max} = 1.000
9524 measured reflections
3852 independent reflections
3080 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 32.8°, θ_{min} = 5.1°
h = −15→18
k = −8→9
l = −23→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.059
S = 0.96
3852 reflections
211 parameters
140 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	−0.03567 (2)	0.75663 (3)	0.03419 (2)	0.01217 (5)	
Cl1	−0.03525 (3)	0.65126 (6)	0.17039 (2)	0.01435 (8)	
Cl2	0.06323 (4)	1.06358 (6)	0.09775 (2)	0.01675 (8)	
Cl3	0.15439 (3)	0.51549 (6)	0.03919 (2)	0.01443 (8)	
N11	0.22343 (13)	0.4646 (2)	0.26811 (9)	0.0150 (3)	
H11	0.1725 (18)	0.522 (3)	0.2289 (13)	0.018*	
C12	0.23527 (14)	0.5451 (2)	0.35078 (10)	0.0141 (3)	
N12	0.17688 (14)	0.7156 (2)	0.35848 (11)	0.0205 (3)	
H12A	0.123 (2)	0.764 (3)	0.3128 (15)	0.025*	
H12B	0.1796 (19)	0.759 (3)	0.4064 (11)	0.025*	
C13	0.31617 (15)	0.4371 (3)	0.42515 (10)	0.0159 (3)	
Cl13	0.33428 (4)	0.53453 (7)	0.53112 (3)	0.02626 (10)	
C14	0.37396 (15)	0.2623 (3)	0.41226 (11)	0.0181 (3)	
H14	0.426057	0.190044	0.462444	0.022*	
C15	0.35667 (15)	0.1878 (3)	0.32427 (11)	0.0168 (3)	
C16	0.28127 (15)	0.2929 (3)	0.25341 (11)	0.0161 (3)	
H16	0.269356	0.245467	0.193687	0.019*	
C17	0.42110 (18)	−0.0020 (3)	0.30815 (12)	0.0247 (4)	
F1	0.3727 (10)	−0.100 (2)	0.2304 (7)	0.039 (3)	0.346 (3)
F2	0.4362 (14)	−0.156 (3)	0.3725 (9)	0.0148 (17)	0.346 (3)
F3	0.5303 (12)	0.049 (3)	0.3161 (10)	0.044 (4)	0.346 (3)
F1A	0.3458 (7)	−0.1196 (15)	0.2373 (5)	0.0245 (12)	0.501 (3)
F2A	0.4471 (11)	−0.133 (2)	0.3777 (7)	0.033 (3)	0.501 (3)
F3A	0.5100 (9)	0.039 (2)	0.2849 (6)	0.041 (2)	0.501 (3)
F1B	0.4390 (13)	0.000 (2)	0.2288 (6)	0.044 (3)	0.153 (3)
F2B	0.4110 (15)	−0.181 (2)	0.3420 (10)	0.045 (4)	0.153 (3)
F3B	0.5484 (9)	0.038 (2)	0.3615 (8)	0.032 (3)	0.153 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01617 (11)	0.00918 (9)	0.01099 (9)	−0.00211 (8)	0.00428 (7)	0.00018 (6)
Cl1	0.0186 (2)	0.01280 (16)	0.01214 (15)	−0.00121 (14)	0.00580 (14)	0.00118 (12)
Cl2	0.0246 (2)	0.01226 (16)	0.01185 (16)	−0.00598 (15)	0.00398 (15)	0.00014 (12)
Cl3	0.01687 (19)	0.01198 (16)	0.01357 (16)	−0.00331 (14)	0.00389 (14)	0.00033 (12)
N11	0.0130 (7)	0.0142 (6)	0.0150 (6)	0.0017 (5)	0.0009 (5)	0.0020 (5)
C12	0.0114 (7)	0.0136 (7)	0.0172 (7)	−0.0022 (6)	0.0045 (6)	−0.0016 (5)
N12	0.0189 (8)	0.0190 (7)	0.0218 (7)	0.0057 (6)	0.0043 (6)	−0.0028 (6)
C13	0.0154 (8)	0.0180 (7)	0.0141 (7)	0.0006 (6)	0.0047 (6)	−0.0004 (6)
Cl13	0.0313 (3)	0.0310 (2)	0.01625 (19)	0.00717 (19)	0.00749 (18)	−0.00405 (16)
C14	0.0172 (8)	0.0191 (8)	0.0170 (7)	0.0040 (7)	0.0046 (6)	0.0041 (6)
C15	0.0184 (9)	0.0147 (7)	0.0181 (7)	0.0026 (6)	0.0070 (7)	0.0018 (6)
C16	0.0180 (8)	0.0143 (7)	0.0165 (7)	−0.0012 (6)	0.0066 (7)	−0.0008 (5)
C17	0.0330 (11)	0.0189 (8)	0.0253 (9)	0.0105 (8)	0.0139 (8)	0.0053 (7)
F1	0.060 (8)	0.043 (6)	0.018 (2)	0.033 (5)	0.019 (4)	0.003 (3)

F2	0.019 (3)	0.005 (3)	0.019 (3)	−0.007 (2)	0.005 (3)	−0.002 (2)
F3	0.051 (7)	0.024 (4)	0.083 (10)	0.008 (5)	0.056 (7)	0.010 (8)
F1A	0.031 (2)	0.0198 (14)	0.025 (2)	0.0052 (15)	0.0116 (15)	−0.0084 (15)
F2A	0.045 (5)	0.015 (3)	0.032 (3)	0.015 (3)	0.002 (3)	0.004 (2)
F3A	0.038 (3)	0.0227 (17)	0.082 (6)	0.000 (2)	0.045 (4)	−0.005 (4)
F1B	0.061 (8)	0.057 (7)	0.017 (4)	0.041 (6)	0.016 (5)	0.004 (4)
F2B	0.035 (8)	0.009 (4)	0.096 (10)	−0.008 (4)	0.028 (8)	−0.018 (6)
F3B	0.017 (4)	0.032 (6)	0.048 (7)	0.009 (4)	0.012 (5)	−0.009 (5)

Geometric parameters (Å, º)

Cu1—Cl1	2.2418 (4)	C14—C15	1.410 (2)
Cu1—Cl2^{i}	2.2868 (4)	C14—H14	0.9500
Cu1—Cl3^{ii}	2.2886 (4)	C15—C16	1.359 (2)
Cu1—Cl2	2.3141 (4)	C15—C17	1.494 (2)
Cu1—Cl3	2.7553 (4)	C16—H16	0.9500
N11—C16	1.349 (2)	C17—F2B	1.263 (13)
N11—C12	1.3578 (19)	C17—F3A	1.286 (9)
N11—H11	0.80 (2)	C17—F2A	1.318 (9)
C12—N12	1.312 (2)	C17—F1	1.322 (11)
C12—C13	1.429 (2)	C17—F1B	1.339 (8)
N12—H12A	0.85 (2)	C17—F3	1.342 (12)
N12—H12B	0.792 (15)	C17—F2	1.363 (11)
C13—C14	1.354 (2)	C17—F1A	1.399 (7)
C13—Cl13	1.7202 (16)	C17—F3B	1.528 (11)
Cl1—Cu1—Cl2^{i}	165.097 (17)	C15—C14—H14	120.1
Cl1—Cu1—Cl3^{ii}	93.655 (14)	C16—C15—C14	119.12 (15)
Cl2^{i}—Cu1—Cl3^{ii}	91.679 (15)	C16—C15—C17	119.94 (15)
Cl1—Cu1—Cl2	89.738 (14)	C14—C15—C17	120.93 (15)
Cl2^{i}—Cu1—Cl2	83.303 (15)	N11—C16—C15	119.84 (15)
Cl3^{ii}—Cu1—Cl2	171.929 (17)	N11—C16—H16	120.1
Cl1—Cu1—Cl3	94.459 (14)	C15—C16—H16	120.1
Cl2^{i}—Cu1—Cl3	99.461 (14)	F3A—C17—F2A	111.6 (8)
Cl3^{ii}—Cu1—Cl3	89.878 (14)	F2B—C17—F1B	118.0 (9)
Cl2—Cu1—Cl3	97.164 (15)	F1—C17—F3	109.0 (8)
Cu1^{i}—Cl2—Cu1	96.698 (15)	F1—C17—F2	105.6 (9)
Cu1^{ii}—Cl3—Cu1	90.121 (14)	F3—C17—F2	102.3 (10)
C16—N11—C12	124.37 (14)	F3A—C17—F1A	106.1 (5)
C16—N11—H11	122.8 (14)	F2A—C17—F1A	104.5 (7)
C12—N11—H11	112.4 (14)	F2B—C17—C15	120.1 (8)
N12—C12—N11	120.11 (15)	F3A—C17—C15	115.7 (7)
N12—C12—C13	124.09 (15)	F2A—C17—C15	110.4 (6)
N11—C12—C13	115.77 (14)	F1—C17—C15	115.2 (6)
C12—N12—H12A	120.3 (14)	F1B—C17—C15	114.3 (4)
C12—N12—H12B	121.0 (16)	F3—C17—C15	111.2 (9)
H12A—N12—H12B	117 (2)	F2—C17—C15	112.5 (7)
C14—C13—C12	120.98 (14)	F1A—C17—C15	107.9 (4)

C14—C13—Cl13	121.70 (13)	F2B—C17—F3B	97.9 (9)
C12—C13—Cl13	117.31 (12)	F1B—C17—F3B	93.4 (7)
C13—C14—C15	119.89 (15)	C15—C17—F3B	106.1 (6)
C13—C14—H14	120.1		
C16—N11—C12—N12	178.72 (16)	C14—C15—C17—F3A	−99.3 (5)
C16—N11—C12—C13	0.7 (2)	C16—C15—C17—F2A	−152.3 (6)
N12—C12—C13—C14	−179.67 (17)	C14—C15—C17—F2A	28.6 (6)
N11—C12—C13—C14	−1.7 (2)	C16—C15—C17—F1	−22.8 (6)
N12—C12—C13—Cl13	1.8 (2)	C14—C15—C17—F1	158.1 (6)
N11—C12—C13—Cl13	179.76 (12)	C16—C15—C17—F1B	27.8 (9)
C12—C13—C14—C15	1.6 (3)	C14—C15—C17—F1B	−151.3 (8)
Cl13—C13—C14—C15	−179.95 (13)	C16—C15—C17—F3	101.9 (7)
C13—C14—C15—C16	−0.3 (3)	C14—C15—C17—F3	−77.2 (7)
C13—C14—C15—C17	178.78 (17)	C16—C15—C17—F2	−143.9 (8)
C12—N11—C16—C15	0.5 (3)	C14—C15—C17—F2	36.9 (8)
C14—C15—C16—N11	−0.7 (3)	C16—C15—C17—F1A	−38.7 (4)
C17—C15—C16—N11	−179.82 (16)	C14—C15—C17—F1A	142.2 (4)
C16—C15—C17—F2B	−121.3 (8)	C16—C15—C17—F3B	129.3 (5)
C14—C15—C17—F2B	59.6 (9)	C14—C15—C17—F3B	−49.9 (5)
C16—C15—C17—F3A	79.8 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···Cl1	0.80 (2)	2.54 (2)	3.2496 (15)	148.6 (18)
N11—H11···Cl3	0.80 (2)	2.92 (2)	3.4332 (14)	123.8 (16)
N12—H12*A*···Cl1	0.85 (2)	2.53 (2)	3.2550 (17)	142.9 (17)
N12—H12*A*···Cl1^{iii}	0.85 (2)	2.70 (2)	3.1823 (15)	117.3 (16)
N12—H12*B*···Cl3^{iv}	0.79 (2)	2.62 (2)	3.3942 (15)	165 (2)

Symmetry codes: (iii) −*x*, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*+3/2, *z*+1/2.