Poly[di-μ_3-chlorido-[μ_2-(3-pyridyl)(4-pyridyl)methanone-κ^2N:N']dicopper(I)]

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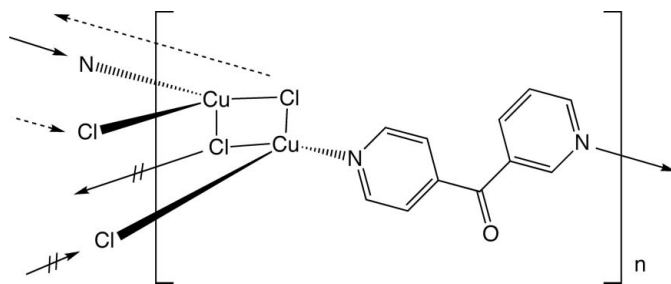
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In the title compound, $[Cu_2Cl_2(C_{11}H_8N_2O)]_n$, stair-like ribbons of formula $[Cu_2Cl_2]_n$ are linked into coordination polymer layers by tethering (3-pyridyl)(4-pyridyl)methanone (3,4′-dpk) ligands. The two distinct Cu^I centres both adopt distorted $CuNCl_3$ tetrahedral coordinations. Individual $[Cu_2Cl_2(3,4′-dpk)]_n$ layers stack in an AB pattern along the c direction by way of weak C—H···O interactions between the pyridyl rings and ketone O atoms.

Related literature

For copper molybdate coordination polymers with (3-pyridyl)-(4-pyridyl)methanone and the synthesis of this ligand, see: Montney & LaDuca (2008). For data-handling software, see: Sheldrick (2003).

Experimental

Crystal data

$[Cu_2Cl_2(C_{11}H_8N_2O)]$	c = 12.339 (2) Å
M_r = 382.17	β = 94.462 (3)°
Monoclinic, $P2_1/c$	V = 1204.9 (4) Å³
a = 3.7765 (7) Å	Z = 4
b = 25.935 (5) Å	Mo $K\alpha$ radiation

μ = 3.96 mm⁻¹	0.22 × 0.14 × 0.08 mm
T = 173 (2) K	

Data collection

Bruker SMART 1K CCD diffractometer	20010 measured reflections
Absorption correction: multi-scan (TWINABS; Sheldrick, 2007)	2794 independent reflections
T_{min} = 0.503, T_{max} = 0.731	2435 reflections with $I > 2\sigma(I)$
	R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039	163 parameters
$wR(F^2)$ = 0.095	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.97 e Å⁻³
2794 reflections	$\Delta\rho_{min}$ = −0.48 e Å⁻³

Table 1
Selected bond lengths (Å).

Cu1—N1	1.995 (3)	Cu2—N2ⁱⁱ	2.002 (3)
Cu1—Cl2	2.2787 (10)	Cu2—Cl1	2.3173 (10)
Cu1—Cl2ⁱ	2.4081 (10)	Cu2—Cl1ⁱ	2.4118 (10)
Cu1—Cl1	2.5854 (11)	Cu2—Cl2ⁱ	2.5343 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1ⁱⁱⁱ	0.93	2.35	3.112 (5)	139

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalMaker* (Palmer, 2007); software used to prepare material for publication: *SHELXL97*.

References

Bruker (2003). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.

Montney, M. R. & LaDuca, R. L. (2008). *J. Solid State Chem.* **181**, 828–836.

Palmer, D. (2007). *Crystal Maker*. CrystalMaker Software, Bicester, Oxfordshire, England.

Sheldrick, G. M. (2003). *CELL-NOW*. University of Göttingen, Germany.

Sheldrick, G. M. (2007). *TWINABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Poly[di-*μ*₃-chlorido-[*μ*₂-(3-pyridyl)(4-pyridyl)methanone-*κ²N:N′*]dicopper(I)]

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S1. Comment

The kinked-donor disposed dipodal tethering ligand (3-pyridyl)(4-pyridyl)methanone (3,4′-dpk) has been rarely utilized for the construction of coordination polymer solids. Two copper molybdate phases incoporating this ligand have been reported recently (Montney & LaDuca, 2008). In an attempt to extend this chemistry into dicarboxylate systems, yellow crystals of the title compound, (I), were obtained.

The asymmetric unit of (I) contains two monovalent copper atoms, two chloride ions and one complete 3,4′-dpk ligand (Fig. 1). The coordination environment at each Cu atom is a distorted {CuCl₃N} tetrahedron (Table 1). The Cu and Cl atoms link into [Cu₂Cl₂]ₙ stair-like ribbons that are oriented parallel to the *a* crystal direction. The Cu···Cu distances across the `steps′ of the stair-like ribbons measure 2.857 (1) Å and 3.153 (1) Å, respectively.
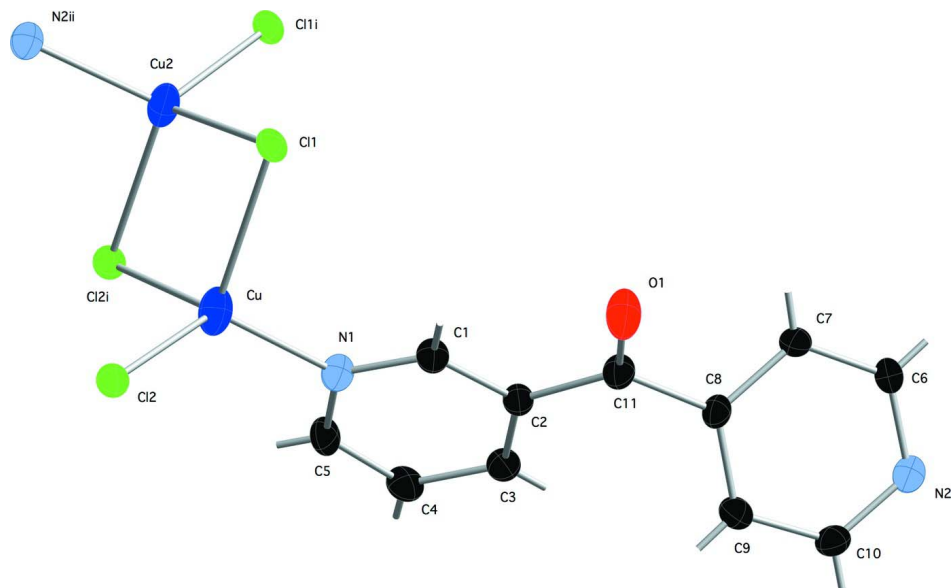
Parallel [Cu₂Cl₂]ₙ ribbons are covalently connected into [Cu₂Cl₂(3,4′-dpk)]ₙ coordination polymer layers, arranged parallel to the *ab* crystal planes, *via* the tethering 3,4′-dpk ligands (Fig. 2). The Cu···Cu contact distances across the di-imine ligands measure 11.573 (3) Å. The dihedral angle between the pyridyl rings within a 3,4′-dpk ligand is 46.53 (17)°. Individual [Cu₂Cl₂(3,4′-dpk)]ₙ layers stack in an *AB* pattern along the *c* crystal direction through weak C—H···O supramolecular interactions between the pyridyl rings and ketone O atoms (Fig. 3), with a C···O contact distance of 3.112 (5) Å (Table 2).

S2. Experimental

All chemicals were obtained commercially with the exception of (3-pyridyl)(4-pyridyl)methanone (Montney & LaDuca, 2008). A mixture of copper(II) chloride dihydrate (63 mg, 0.37 mmol), phthalic acid (61 mg, 0.37 mmol), (3-pyridyl)(4-pyridyl)methanone (136 mg, 0.74 mmol) and 10.0 g water (555 mmol) was placed in a 23 ml Teflon-lined Parr acid digestion bomb, which was then heated under autogenous pressure at 393 K for 48 h. Yellow–orange blocks of (I) were obtained.

S3. Refinement

Reflection data were collected on a non-merohedrally twinned crystal. The twin law was determined with *CELL-NOW* (Sheldrick, 2003). The structure was solved and refined using reflections from only the major twin component, whose reflection file was generated using *TWINABS* (Sheldrick, 2007). All H atoms bound to C atoms were placed in calculated positions, with C—H = 0.95 Å and refined in riding mode with $U_{iso} = 1.2U_{eq}(C)$.

Figure 1

Asymmetric unit of (I), expanded to show the metal coordination spheres, showing 50% probability ellipsoids. Hydrogen atom positions are shown as gray sticks. Symmetry codes: (1) x - 1, y, z (ii) -x, y - 1/2, -z + 1/2

Figure 2

A single [Cu$_2$Cl$_2$(3,4′-dpk)]$_n$ layer in (I) formed by the linkage of [Cu$_2$Cl$_2$]$_n$ ladders through the diimine ligands.
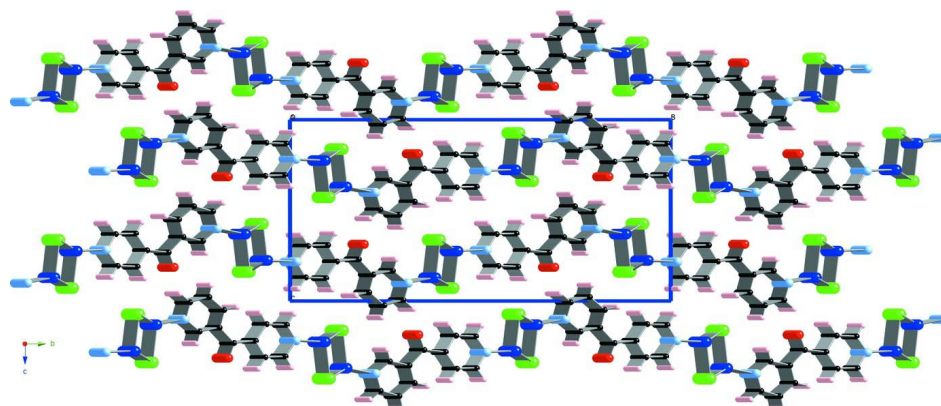
Figure 3

Packing diagram illustrating the *AB* layer stacking pattern, which forms the 3-D crystal structure of (I) through weak C—H⋯O interactions between pyridyl rings and ketone O atoms.

Poly[di-*μ₃*-chlorido-[*μ₂*-(3-pyridyl)(4-pyridyl)methanone- *κ²*N:N′]dicopper(I)]

Crystal data

[Cu₂Cl₂(C₁₁H₈N₂O)]
$M_r = 382.17$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 3.7765 (7)$ Å
$b = 25.935 (5)$ Å
$c = 12.339 (2)$ Å
$β = 94.462 (3)°$
$V = 1204.9 (4)$ Å³
$Z = 4$

$F(000) = 752$
$D_x = 2.107$ Mg m⁻³
Mo $Kα$ radiation, $λ = 0.71073$ Å
Cell parameters from 20010 reflections
$θ = 1.6–28.3°$
$μ = 3.96$ mm⁻¹
$T = 173$ K
Block, yellow
$0.22 × 0.14 × 0.08$ mm

Data collection

Bruker SMART 1K CCD
    diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
    (TWINABS; Sheldrick, 2007)
$T_{min} = 0.503$, $T_{max} = 0.731$

20010 measured reflections
2794 independent reflections
2435 reflections with $I > 2σ(I)$
$R_{int} = 0.042$
$θ_{max} = 28.3°$, $θ_{min} = 1.6°$
$h = −5→4$
$k = 0→34$
$l = 0→16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2σ(F^2)] = 0.039$
$wR(F^2) = 0.095$
$S = 1.06$
2794 reflections
163 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
$w = 1/[σ^2(F_o^2) + (0.0339P)^2 + 4.4918P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(Δ/σ)_{max} = 0.001$
$Δρ_{max} = 0.97$ e Å⁻³
$Δρ_{min} = −0.48$ 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 for the major twin component. 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 (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Cu1	0.30817 (14)	0.633401 (18)	0.12987 (4)	0.03284 (15)
Cu2	−0.09246 (14)	0.576023 (18)	0.27566 (4)	0.03282 (15)
Cl1	0.4078 (2)	0.62217 (3)	0.33820 (6)	0.01995 (17)
Cl2	0.7724 (2)	0.58732 (3)	0.07265 (7)	0.02118 (18)
N1	0.1879 (8)	0.70719 (11)	0.0999 (2)	0.0217 (6)
C2	0.2012 (9)	0.79762 (13)	0.1460 (3)	0.0186 (6)
N2	0.1356 (8)	0.99919 (11)	0.2175 (2)	0.0228 (6)
C8	0.2454 (9)	0.89246 (12)	0.2191 (3)	0.0193 (7)
C7	0.1332 (10)	0.91779 (14)	0.3097 (3)	0.0237 (7)
H7	0.0973	0.8995	0.3728	0.028*
C1	0.2845 (9)	0.74576 (13)	0.1677 (3)	0.0205 (7)
H1	0.4139	0.7378	0.2327	0.025*
O1	0.4939 (9)	0.82138 (10)	0.3137 (2)	0.0371 (7)
C9	0.2995 (9)	0.92152 (14)	0.1272 (3)	0.0224 (7)
H9	0.3696	0.9058	0.0646	0.027*
C5	−0.0002 (10)	0.71977 (14)	0.0055 (3)	0.0238 (7)
H5	−0.0729	0.6934	−0.0423	0.029*
C4	−0.0885 (10)	0.76977 (14)	−0.0230 (3)	0.0236 (7)
H4	−0.2124	0.7768	−0.0895	0.028*
C3	0.0094 (9)	0.80956 (13)	0.0486 (3)	0.0210 (7)
H3	−0.0523	0.8435	0.0316	0.025*
C10	0.2469 (9)	0.97448 (13)	0.1308 (3)	0.0216 (7)
H10	0.2911	0.9939	0.0699	0.026*
C6	0.0756 (10)	0.97045 (14)	0.3052 (3)	0.0252 (7)
H6	−0.0083	0.9867	0.3653	0.030*
C11	0.3264 (10)	0.83580 (13)	0.2312 (3)	0.0218 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0365 (3)	0.0196 (2)	0.0417 (3)	0.00451 (19)	−0.0013 (2)	−0.0024 (2)
Cu2	0.0436 (3)	0.0188 (2)	0.0359 (3)	−0.0030 (2)	0.0024 (2)	−0.00250 (19)
Cl1	0.0204 (4)	0.0227 (4)	0.0165 (4)	−0.0004 (3)	−0.0001 (3)	−0.0049 (3)
Cl2	0.0234 (4)	0.0203 (4)	0.0197 (4)	0.0012 (3)	0.0005 (3)	−0.0002 (3)
N1	0.0223 (15)	0.0191 (14)	0.0232 (15)	0.0003 (11)	−0.0024 (11)	0.0000 (11)

C2	0.0198 (16)	0.0178 (15)	0.0181 (15)	0.0006 (12)	0.0008 (12)	−0.0004 (12)
N2	0.0243 (15)	0.0187 (14)	0.0251 (15)	−0.0012 (11)	0.0001 (12)	−0.0002 (12)
C8	0.0227 (17)	0.0155 (15)	0.0191 (16)	−0.0016 (12)	−0.0020 (13)	−0.0007 (12)
C7	0.035 (2)	0.0209 (17)	0.0149 (16)	−0.0059 (14)	0.0029 (14)	−0.0002 (13)
C1	0.0234 (17)	0.0195 (16)	0.0177 (16)	0.0010 (13)	−0.0035 (13)	0.0006 (13)
O1	0.0581 (19)	0.0229 (13)	0.0270 (14)	0.0042 (13)	−0.0178 (13)	−0.0015 (11)
C9	0.0263 (18)	0.0235 (17)	0.0174 (16)	0.0006 (14)	0.0021 (13)	−0.0013 (13)
C5	0.0278 (18)	0.0210 (16)	0.0219 (17)	−0.0008 (14)	−0.0021 (14)	−0.0069 (14)
C4	0.0273 (19)	0.0265 (18)	0.0162 (16)	0.0018 (14)	−0.0040 (13)	0.0006 (13)
C3	0.0235 (17)	0.0200 (16)	0.0192 (16)	0.0032 (13)	0.0002 (13)	0.0022 (13)
C10	0.0233 (17)	0.0224 (17)	0.0190 (16)	−0.0014 (13)	0.0009 (13)	0.0043 (13)
C6	0.035 (2)	0.0191 (17)	0.0219 (17)	−0.0034 (14)	0.0056 (15)	−0.0053 (14)
C11	0.0265 (18)	0.0185 (16)	0.0197 (16)	0.0001 (13)	−0.0025 (13)	0.0010 (13)

Geometric parameters (Å, º)

Cu1—N1	1.995 (3)	C8—C9	1.390 (5)
Cu1—Cl2	2.2787 (10)	C8—C7	1.391 (5)
Cu1—Cl2[i]	2.4081 (10)	C8—C11	1.506 (5)
Cu1—Cl1	2.5854 (11)	C7—C6	1.383 (5)
Cu2—N2[ii]	2.002 (3)	C7—H7	0.9300
Cu2—Cl1	2.3173 (10)	C1—H1	0.9300
Cu2—Cl1[i]	2.4118 (10)	O1—C11	1.216 (4)
Cu2—Cl2[i]	2.5343 (11)	C9—C10	1.389 (5)
N1—C1	1.336 (4)	C9—H9	0.9300
N1—C5	1.356 (5)	C5—C4	1.378 (5)
C2—C3	1.389 (5)	C5—H5	0.9300
C2—C1	1.403 (5)	C4—C3	1.390 (5)
C2—C11	1.494 (5)	C4—H4	0.9300
N2—C10	1.343 (5)	C3—H3	0.9300
N2—C6	1.348 (5)	C10—H10	0.9300
N2—Cu2[iii]	2.002 (3)	C6—H6	0.9300
N1—Cu1—Cl2	127.98 (9)	C10—N2—Cu2[iii]	122.7 (2)
N1—Cu1—Cl2[i]	104.34 (9)	C6—N2—Cu2[iii]	119.9 (2)
Cl2—Cu1—Cl2[i]	107.34 (4)	C9—C8—C7	118.2 (3)
N1—Cu1—Cl1	107.80 (9)	C9—C8—C11	124.6 (3)
Cl2—Cu1—Cl1	101.13 (3)	C7—C8—C11	117.0 (3)
Cl2[i]—Cu1—Cl1	106.83 (3)	C6—C7—C8	119.4 (3)
N1—Cu1—Cu2	119.49 (9)	C6—C7—H7	120.3
Cl2—Cu1—Cu2	112.32 (3)	C8—C7—H7	120.3
Cl2[i]—Cu1—Cu2	56.78 (3)	N1—C1—C2	123.5 (3)
Cl1—Cu1—Cu2	50.09 (2)	N1—C1—H1	118.2
N2[ii]—Cu2—Cl1	124.54 (9)	C2—C1—H1	118.2
N2[ii]—Cu2—Cl1[i]	114.36 (9)	C10—C9—C8	118.7 (3)
Cl1—Cu2—Cl1[i]	105.97 (4)	C10—C9—H9	120.7
N2[ii]—Cu2—Cl2[i]	98.38 (9)	C8—C9—H9	120.7
Cl1—Cu2—Cl2[i]	111.46 (3)	N1—C5—C4	123.1 (3)

Cl1^i—Cu2—Cl2^i	99.00 (3)	N1—C5—H5	118.5
N2^{ii}—Cu2—Cu1	126.42 (9)	C4—C5—H5	118.5
Cl1—Cu2—Cu1	58.85 (3)	C5—C4—C3	119.3 (3)
Cl1^i—Cu2—Cu1	114.14 (3)	C5—C4—H4	120.3
Cl2^i—Cu2—Cu1	52.64 (3)	C3—C4—H4	120.3
Cu2—Cl1—Cu2^{iv}	105.97 (4)	C2—C3—C4	118.7 (3)
Cu2—Cl1—Cu1	71.05 (3)	C2—C3—H3	120.7
Cu2^{iv}—Cl1—Cu1	78.15 (3)	C4—C3—H3	120.7
Cu1—Cl2—Cu1^{iv}	107.34 (4)	N2—C10—C9	123.5 (3)
Cu1—Cl2—Cu2^{iv}	81.67 (3)	N2—C10—H10	118.3
Cu1^{iv}—Cl2—Cu2^{iv}	70.58 (3)	C9—C10—H10	118.3
C1—N1—C5	117.2 (3)	N2—C6—C7	122.9 (3)
C1—N1—Cu1	123.7 (2)	N2—C6—H6	118.6
C5—N1—Cu1	119.1 (2)	C7—C6—H6	118.6
C3—C2—C1	118.2 (3)	O1—C11—C2	120.1 (3)
C3—C2—C11	125.2 (3)	O1—C11—C8	118.1 (3)
C1—C2—C11	116.6 (3)	C2—C11—C8	121.8 (3)
C10—N2—C6	117.3 (3)		
N1—Cu1—Cu2—N2^{ii}	158.68 (15)	Cl2—Cu1—N1—C1	−95.8 (3)
Cl2—Cu1—Cu2—N2^{ii}	−26.27 (12)	Cl2^i—Cu1—N1—C1	138.1 (3)
Cl2^i—Cu1—Cu2—N2^{ii}	70.41 (11)	Cl1—Cu1—N1—C1	24.8 (3)
Cl1—Cu1—Cu2—N2^{ii}	−112.18 (12)	Cu2—Cu1—N1—C1	78.4 (3)
N1—Cu1—Cu2—Cl1	−89.14 (10)	Cl2—Cu1—N1—C5	83.7 (3)
Cl2—Cu1—Cu2—Cl1	85.91 (4)	Cl2^i—Cu1—N1—C5	−42.4 (3)
Cl2^i—Cu1—Cu2—Cl1	−177.41 (4)	Cl1—Cu1—N1—C5	−155.8 (3)
N1—Cu1—Cu2—Cl1^i	5.53 (10)	Cu2—Cu1—N1—C5	−102.1 (3)
Cl2—Cu1—Cu2—Cl1^i	−179.41 (4)	C9—C8—C7—C6	0.8 (5)
Cl2^i—Cu1—Cu2—Cl1^i	−82.74 (4)	C11—C8—C7—C6	176.2 (3)
Cl1—Cu1—Cu2—Cl1^i	94.67 (4)	C5—N1—C1—C2	0.1 (5)
N1—Cu1—Cu2—Cl2^i	88.27 (10)	Cu1—N1—C1—C2	179.6 (3)
Cl2—Cu1—Cu2—Cl2^i	−96.67 (4)	C3—C2—C1—N1	−0.3 (5)
Cl1—Cu1—Cu2—Cl2^i	177.41 (4)	C11—C2—C1—N1	179.3 (3)
N2^{ii}—Cu2—Cl1—Cu2^{iv}	44.13 (12)	C7—C8—C9—C10	1.4 (5)
Cl1^i—Cu2—Cl1—Cu2^{iv}	180.0	C11—C8—C9—C10	−173.6 (3)
Cl2^i—Cu2—Cl1—Cu2^{iv}	−73.30 (4)	C1—N1—C5—C4	0.9 (6)
Cu1—Cu2—Cl1—Cu2^{iv}	−71.09 (3)	Cu1—N1—C5—C4	−178.6 (3)
N2^{ii}—Cu2—Cl1—Cu1	115.22 (11)	N1—C5—C4—C3	−1.7 (6)
Cl1^i—Cu2—Cl1—Cu1	−108.91 (3)	C1—C2—C3—C4	−0.5 (5)
Cl2^i—Cu2—Cl1—Cu1	−2.21 (3)	C11—C2—C3—C4	179.9 (3)
N1—Cu1—Cl1—Cu2	113.91 (9)	C5—C4—C3—C2	1.5 (5)
Cl2—Cu1—Cl1—Cu2	−109.88 (4)	C6—N2—C10—C9	0.5 (5)
Cl2^i—Cu1—Cl1—Cu2	2.26 (3)	Cu2^{iii}—N2—C10—C9	175.9 (3)
N1—Cu1—Cl1—Cu2^{iv}	−134.42 (9)	C8—C9—C10—N2	−2.1 (6)
Cl2—Cu1—Cl1—Cu2^{iv}	1.79 (3)	C10—N2—C6—C7	1.8 (6)
Cl2^i—Cu1—Cl1—Cu2^{iv}	113.93 (3)	Cu2^{iii}—N2—C6—C7	−173.7 (3)
Cu2—Cu1—Cl1—Cu2^{iv}	111.67 (3)	C8—C7—C6—N2	−2.5 (6)
N1—Cu1—Cl2—Cu1^{iv}	55.05 (12)	C3—C2—C11—O1	−179.8 (4)

Cl2^i—Cu1—Cl2—Cu1^iv	180.0	C1—C2—C11—O1	0.6 (5)
Cl1—Cu1—Cl2—Cu1^iv	−68.25 (4)	C3—C2—C11—C8	1.3 (5)
Cu2—Cu1—Cl2—Cu1^iv	−119.49 (3)	C1—C2—C11—C8	−178.3 (3)
N1—Cu1—Cl2—Cu2^iv	121.61 (11)	C9—C8—C11—O1	131.7 (4)
Cl2^i—Cu1—Cl2—Cu2^iv	−113.44 (3)	C7—C8—C11—O1	−43.4 (5)
Cl1—Cu1—Cl2—Cu2^iv	−1.69 (3)	C9—C8—C11—C2	−49.4 (5)
Cu2—Cu1—Cl2—Cu2^iv	−52.93 (3)	C7—C8—C11—C2	135.5 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^v	0.93	2.35	3.112 (5)	139

Symmetry code: (v) $x-1, -y+3/2, z-1/2$.