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Crystal structure of a chloride-bridged copper(II) dimer: piperazine-1,4-dium bis(di-μ-chlorido-bis[(4-carboxypyridine-2-carboxylato-κ^2N,O^2)-chloridocuprate(II)]

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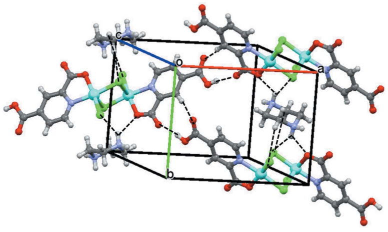
Crystals of a new dimeric chloride-bridged cuprate(II) derived from pyridine-2,4-dicarboxylic acid were obtained solvothermally in the presence of piperazine and hydrochloric acid. The crystal structure determination of the title salt, $(C_4H_{12}N_2)[Cu_2(C_7H_4NO_4)_2Cl_4]$, revealed one of the carboxyl groups of the original pyridine-2,4-dicarboxylic acid ligand to be protonated, whereas the other is deprotonated and binds together with the pyridine N atom to the Cu^{II} atom. The coordination environment of the Cu^{II} atom is distorted square-pyramidal. One of the chloride ligands bridges two metal cations to form a centrosymmetric dimer with two different Cu—Cl distances of 2.2632 (8) and 2.7853 (8) Å, whereby the longer distance is associated with the apical ligand. The remaining chloride ligand is terminal at one of the basal positions, with a distance of 2.2272 (9) Å. In the crystal, the dimers are linked by intermolecular O—H···O hydrogen bonds, together with N—H···O and N—H···Cl interactions involving the centrosymmetric organic cation, into a three-dimensional supramolecular network. Further but weaker C—H···O and C—H···Cl interactions consolidate the packing.



1. Chemical context

In recent times, research on coordination polymers, popularly known as metal–organic frameworks (MOFs), have received great attention, not only for their potential applications in the area of gas storage, ion-exchange, non-linear optics, molecular sieves, catalysis, magnetism, and molecular sensing (Yaghi *et al.*, 2003; Ockwig *et al.*, 2005; Wang *et al.*, 2005; Carlucci *et al.*, 2003; Hill *et al.*, 2005), but also for their rich structural chemistry (Li *et al.*, 2016; Eddaoudi *et al.*, 2015). In the design of compounds with metal–organic frameworks, versatile carboxylate ligands, derived from 1,4-benzenedicarboxylic acid, 1,3,5-benzenetricarboxylic acid, 1,2,4,5-benzenetetracarboxylic acid or pyridine-2,4-dicarboxylic acid, have frequently been used owing to their abundant carboxylate groups possessing high affinity to metal cations (Li *et al.*, 2004; Shi *et al.*, 2004; Gutschke *et al.*, 2001; Tao *et al.*, 2000). A number of novel metal–organic frameworks have been constructed using di- or multicarboxylate ligands as linkers. Most of the reported MOF materials have been synthesized using solvothermal or hydrothermal synthetic conditions, often by using sealed autoclaves. These techniques have also been found to play an important role in preparing robust and stable inorganic compounds with open frameworks (Rao *et al.*, 2001; Eddaoudi *et al.*, 2001). The fact that the solubility of the reactants increases under hydrothermal methods makes the reaction more likely to occur at lower temperatures, with the formation of polymeric units through molecular building blocks (Zhao *et al.*, 2007). Small changes in one or more of the reaction variables, such as temperature, time, pH or the solvent type, can have a profound influence on the product. In some cases, organic amines or alkylammonium cations are used as templates and/or structure-directing agents in the crystallization process of framework solids (Jiang *et al.*, 1998; Cheetham *et al.*, 1999). In the course of our investigations, we were interested in using pyridine-2,4-dicarboxylic acid as a source of *N*- and *O*-donors, in synthesizing a coordination polymer in an acidic medium under solvothermal conditions and in the presence of piperazine as an organic amine. In this context we report on the synthesis and crystal structure of the title compound $(C_4H_{12}N_2)[Cu_2(C_7H_4NO_4)_2Cl_4]$, (I).

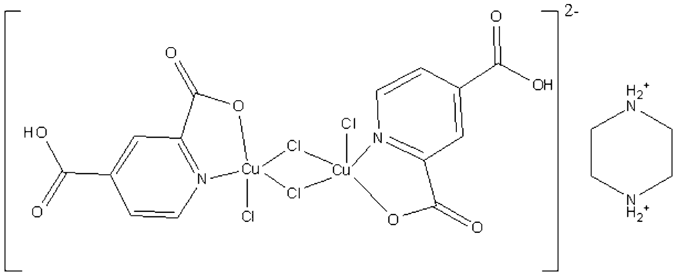


Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H3···O4^{i}	0.82	1.79	2.603 (3)	171
N2—H2*A*···Cl1^{ii}	0.89	2.78	3.562 (3)	147
N2—H2*A*···O3^{ii}	0.89	2.22	2.861 (3)	129
N2—H2*B*···Cl1^{iii}	0.89	2.69	3.414 (3)	139
N2—H2*B*···Cl2^{iii}	0.89	2.69	3.360 (3)	133
C2—H2···O2^{iv}	0.93	2.49	3.402 (4)	169
C4—H12···O2^{v}	0.93	2.56	3.362 (4)	145
C5—H13···Cl2	0.93	2.71	3.269 (3)	119
C8—H27*A*···Cl1^{vi}	0.97	2.72	3.561 (3)	146
C8—H27*B*···Cl2^{vii}	0.97	2.81	3.599 (3)	139
C9—H26*A*···O2^{viii}	0.97	2.56	3.509 (4)	165
C9—H26*B*···Cl1^{vi}	0.97	2.93	3.713 (3)	139
C9—H26*B*···Cl2^{iii}	0.97	2.93	3.491 (4)	118

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $x, y-1, z$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+2, y-\frac{3}{2}, -z+\frac{1}{2}$; (vii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (viii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

2. Structural commentary

The molecular structure of (I) showing the numbering scheme is presented in Fig. 1. The copper(II) atom is chelated by the O atom (O3) of the deprotonated carboxylic group and the pyridine N atom (N1) of the organic ligand, forming a five-membered chelate ring Cu1–N1–C1–C6–O3. Two bridging and one terminal chlorido ligands complete the distorted square-pyramidal coordination of the metal cation. The arrangement of the chlorido ligands is such that Cl1 is doubly bridging the two metal cations into a centrosymmetric dimer through edge-sharing. The apical Cu—Cl1($-x+2$, $-y+2$, $-z+1$) bond length of 2.7853 (9) Å is significantly longer than the other bridging Cu—Cl bond with a length of 2.2632 (8) Å. The square plane is formed by N1 and O3, both from the pyridine-2,4-dicarboxylate anion, Cl1 from the bridging chlorido ligand and Cl2 of the terminal chlorido ligand [2.2272 (9) Å]. This type of coordination has been previously described as a transition state between 4- and 5-coordinate (Qi *et al.*, 2009). The distortion index (τ) assuming a square-pyramidal environment was calculated as 0.08 using the formula, $\tau = (\beta - \alpha)/60$ (α, β are the largest valence angles) proposed by Addison *et al.* (1984), which indicates only slight distortions from the ideal value where $\tau = 0$. The Cu···Cu distance in the dimer is 3.5946 (9) Å, with an Cu—Cl—Cu bond angle of 90.19 (3)° and a Cl···Cl separation of 3.5831 (14) Å. The Cu—N and Cu—O bond lengths are 2.013 (2) and 1.963 (2) Å, respectively, and are in good agreement with similar compounds reported in the literature (Goddard *et al.*, 1990; Tynan *et al.*, 2005; Han *et al.*, 2008; Liu *et al.*, 2009; Qi *et al.*, 2009). The chelate angle O3—Cu—N1 of 81.34 (9)° is, as expected, smaller than the N1—Cu—Cl1 and O3—Cu—Cl2 bond angles of 170.22 (7) and 165.23 (8)°, respectively. The inorganic anion has a charge of −2 that is compensated by the incorporation of a fully protonated piperazine molecule in the structure. The latter is located about an inversion centre.

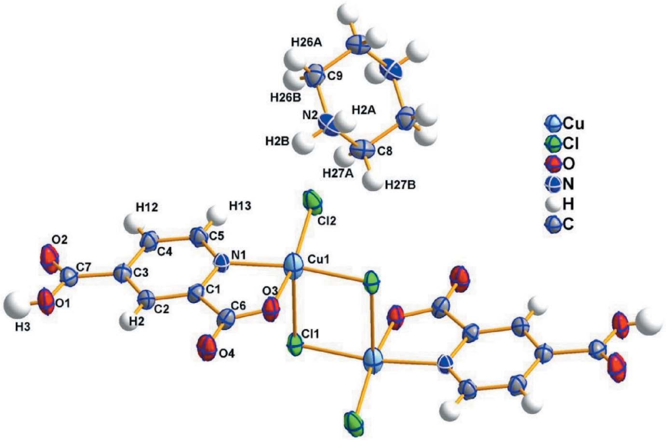


Figure 1
The molecular structures of the cationic and anionic components of (I). Displacement ellipsoids are drawn at the 50% probability level. The non-labelled atoms are related to the labelled atoms by $-x+2, -y+2, -z+1$;.

3. Supramolecular features

The centrosymmetric dimers are linked by pairs of (carboxyl)-O1—H3···O4(carboxylate) hydrogen bonds to form sheets parallel (100). The protonated centrosymmetric amine cations are situated between the sheets and are connected through N2—H···O2 interactions to one of the carbonyl oxygen atoms and various N—H···Cl interactions into a three-dimensional network (Table 1, Fig. 2). The carbonyl oxygen atom O2 also

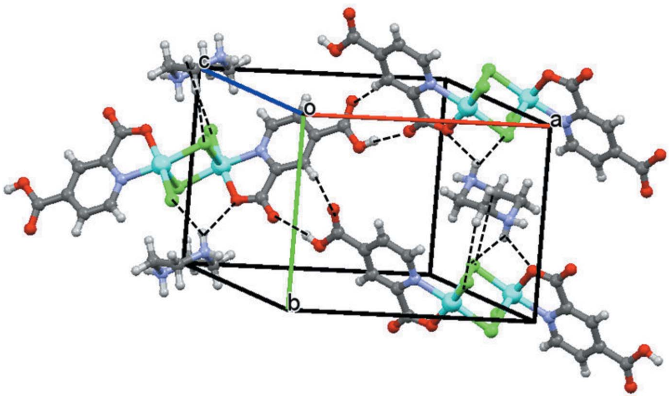


Figure 2
The crystal structure of (I), showing O—H···O, N—H···O and N—H···Cl hydrogen-bonding interactions as dashed lines (see Table 1 for numerical details).

acts as a hydrogen-bond acceptor from pyridyl C—H groups (C2—H2···O2 and C4—H12···O2). These interactions, together with C—H···Cl interactions, further stabilize the three-dimensional supramolecular network structure.

4. Database survey

There are several copper(II) dimeric compounds in which the copper atoms are bridged by chlorido ligands (Marsh *et al.*, 1983; Puschmann *et al.*, 2001; Li *et al.*, 2006; Lee, *et al.*, 2008; Han *et al.*, 2008; Øien *et al.*, 2013; Choubey *et al.*, 2015; Golchoubian & Nateghi 2016; Liu *et al.*, 2009). A search of the Cambridge Structural Database (Version 5.38, November 2016; Groom *et al.*, 2016), revealed numerous di-μ-chlorido bridged copper(II) compounds constructed with ligands having -*N,O*- donor atoms (Kapoor *et al.*, 2002, 2004; Damous *et al.*, 2013; Lumb *et al.*, 2013; Smolentsev *et al.*, 2014; Qureshi *et al.*, 2016). However, the search did not reveal related complexes derived from pyridine-2,4-dicarboxylic acid and piperazine.

5. Synthesis and crystallization

The syntheses were carried out in Ace pressure tubes (15 cm^3) and heated in programmable ovens. The reagents used for syntheses were obtained from Aldrich (Analar grade) and used without further purification. In a typical synthesis of (I), $Cu(CH_3COO)_2 \cdot 2H_2O$ (0.1996 g, 1.0 mmol) was stirred together with pyridine-2,4-dicarboxylic acid (0.1671 g, 1.0 mmol) in 3.3 cm^3 of *n*-butanol. This was followed by the addition of piperazine (0.940 g, 1.0 mmol) and the pH of the solution was adjusted to 2 by dropwise addition of 0.16 cm^3 of conc. HCl. The resultant mixture was homogenized for 15 min before transferring into the reaction vessel and heated in an oven at 393 K for 48 h. The product, a crop of bluish crystalline material, was washed with distilled water and air-dried.

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_4H_{12}N_2)[Cu_2(C_7H_4NO_4)_2Cl_4]$
M_r	689.26
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	11.639 (3), 9.224 (2), 11.423 (3)
β (°)	105.211 (3)
V (Å^3)	1183.4 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.30
Crystal size (mm)	0.05 × 0.02 × 0.02
Data collection	
Diffractometer	Bruker *SMART APEX* CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.946, 0.955
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14235, 2923, 2392
R_{int}	0.050
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.127, 0.86
No. of reflections	2923
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.31

Computer programs: *SMART* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were treated as riding atoms, with C—H distances of 0.93 Å (aromatic) and 0.97 Å (aliphatic), and with $U_{iso}(H) = 1.2U_{eq}(C)$. N- and O-bound H atoms were located in difference maps and were refined with N—H distances of 0.89 Å and O—H distances of 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$, respectively.

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supporting information

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Crystal structure of a chloride-bridged copper(II) dimer: piperazine-1,4-dium bis(di-μ-chlorido-bis[(4-carboxypyridine-2-carboxylato-κ^2N,O^2)chloridocuprate(II)]

Bassey Enyi Inah, Ayi Anyama Ayi and Amit Adhikary

Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Piperazine-1,4-dium bis(di-μ-chlorido-bis[(4-carboxypyridine-2-carboxylato-κ^2N,O^2)chloridocuprate(II)]

Crystal data

$(C_4H_{12}N_2)[Cu_2(C_7H_4NO_4)_2Cl_4]$
M_r = 689.26
Monoclinic, $P2_1/c$
a = 11.639 (3) Å
b = 9.224 (2) Å
c = 11.423 (3) Å
β = 105.211 (3)°
V = 1183.4 (5) Å^3
Z = 2
$F(000)$ = 692
D_x = 1.934 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1016 reflections
θ = 2.9–26.8°
μ = 2.30 mm^{-1}
T = 298 K
Rod, blue
0.05 × 0.02 × 0.02 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.946, T_{max} = 0.955
14235 measured reflections
2923 independent reflections
2392 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 28.3°, θ_{min} = 2.9°
$h = -15\rightarrow15$
$k = -12\rightarrow12$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.127
S = 0.86
2923 reflections
164 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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}
Cu1	0.84456 (3)	1.01123 (4)	0.42216 (3)	0.02632 (15)
Cl1	0.99944 (6)	1.14015 (7)	0.39127 (7)	0.02963 (19)
Cl2	0.82884 (8)	0.86943 (9)	0.26090 (7)	0.0431 (2)
O3	0.82154 (19)	1.1592 (2)	0.5374 (2)	0.0326 (5)
O4	0.7301 (2)	1.2063 (2)	0.6797 (2)	0.0411 (6)
N1	0.7122 (2)	0.9149 (2)	0.4767 (2)	0.0244 (5)
O1	0.4230 (2)	0.8203 (3)	0.7170 (2)	0.0412 (6)
H3	0.379334	0.776566	0.750692	0.062*
C6	0.7489 (2)	1.1293 (3)	0.5993 (3)	0.0259 (6)
N2	0.9556 (2)	0.0777 (3)	0.0881 (2)	0.0358 (6)
H2A	0.959588	0.169430	0.065288	0.043*
H2B	0.926778	0.077335	0.152968	0.043*
C1	0.6847 (3)	0.9859 (3)	0.5683 (3)	0.0246 (6)
O2	0.4234 (2)	0.6091 (3)	0.6208 (2)	0.0468 (6)
C2	0.6029 (2)	0.9326 (3)	0.6261 (3)	0.0261 (6)
H2	0.584506	0.983758	0.688974	0.031*
C8	1.0765 (3)	0.0148 (3)	0.1210 (3)	0.0323 (7)
H27A	1.073784	−0.081047	0.155093	0.039*
H27B	1.128410	0.074758	0.182456	0.039*
C7	0.4583 (3)	0.7319 (3)	0.6429 (3)	0.0310 (6)
C4	0.5776 (3)	0.7273 (3)	0.4928 (3)	0.0308 (6)
H12	0.542510	0.638592	0.465717	0.037*
C5	0.6597 (3)	0.7892 (3)	0.4394 (3)	0.0294 (6)
H13	0.678695	0.741211	0.375346	0.035*
C3	0.5487 (3)	0.7998 (3)	0.5872 (3)	0.0268 (6)
C9	0.8733 (3)	−0.0041 (3)	−0.0119 (3)	0.0367 (7)
H26A	0.796776	0.044487	−0.034859	0.044*
H26B	0.861083	−0.100761	0.016075	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0282 (2)	0.0222 (2)	0.0335 (2)	−0.00475 (12)	0.01701 (17)	−0.00548 (13)
Cl1	0.0306 (4)	0.0252 (3)	0.0368 (4)	−0.0053 (3)	0.0155 (3)	0.0021 (3)
Cl2	0.0595 (5)	0.0385 (4)	0.0410 (5)	−0.0166 (4)	0.0305 (4)	−0.0152 (3)
O3	0.0350 (11)	0.0255 (10)	0.0437 (12)	−0.0075 (9)	0.0215 (10)	−0.0092 (9)
O4	0.0424 (13)	0.0372 (12)	0.0520 (14)	−0.0066 (10)	0.0272 (11)	−0.0194 (10)
N1	0.0249 (11)	0.0239 (12)	0.0270 (11)	−0.0007 (9)	0.0112 (9)	−0.0022 (9)
O1	0.0441 (14)	0.0401 (13)	0.0497 (14)	−0.0112 (11)	0.0306 (12)	−0.0032 (11)

C6	0.0219 (13)	0.0217 (13)	0.0348 (15)	−0.0001 (10)	0.0086 (11)	−0.0051 (11)
N2	0.0454 (15)	0.0311 (14)	0.0334 (13)	0.0120 (12)	0.0150 (12)	0.0001 (11)
C1	0.0209 (12)	0.0247 (14)	0.0281 (14)	0.0024 (10)	0.0064 (11)	−0.0005 (10)
O2	0.0573 (16)	0.0355 (12)	0.0581 (16)	−0.0167 (11)	0.0337 (13)	−0.0040 (11)
C2	0.0238 (13)	0.0291 (14)	0.0264 (13)	−0.0003 (11)	0.0085 (11)	−0.0007 (11)
C8	0.0422 (18)	0.0228 (14)	0.0280 (15)	0.0016 (12)	0.0027 (14)	−0.0002 (11)
C7	0.0290 (14)	0.0344 (16)	0.0291 (14)	−0.0046 (12)	0.0068 (12)	0.0058 (12)
C4	0.0309 (15)	0.0276 (14)	0.0350 (15)	−0.0075 (12)	0.0106 (13)	−0.0022 (12)
C5	0.0320 (15)	0.0288 (15)	0.0300 (14)	−0.0037 (12)	0.0130 (12)	−0.0053 (11)
C3	0.0240 (13)	0.0276 (14)	0.0291 (14)	0.0002 (11)	0.0076 (11)	0.0037 (11)
C9	0.0313 (17)	0.0374 (18)	0.0416 (19)	0.0024 (12)	0.0099 (15)	0.0037 (13)

Geometric parameters (Å, º)

Cu1—O3	1.963 (2)	N2—H2B	0.8900
Cu1—N1	2.013 (2)	C1—C2	1.384 (4)
Cu1—Cl2	2.2272 (9)	O2—C7	1.207 (4)
Cu1—Cl1	2.2632 (8)	C2—C3	1.396 (4)
Cu1—Cl1$^{\text{i}}$	2.7853 (9)	C2—H2	0.9300
O3—C6	1.267 (3)	C8—C9$^{\text{ii}}$	1.512 (5)
O4—C6	1.225 (3)	C8—H27A	0.9700
N1—C5	1.327 (4)	C8—H27B	0.9700
N1—C1	1.343 (4)	C7—C3	1.502 (4)
O1—C7	1.316 (4)	C4—C3	1.383 (4)
O1—H3	0.8200	C4—C5	1.385 (4)
C6—C1	1.515 (4)	C4—H12	0.9300
N2—C8	1.476 (4)	C5—H13	0.9300
N2—C9	1.490 (4)	C9—H26A	0.9700
N2—H2A	0.8900	C9—H26B	0.9700
O3—Cu1—N1	81.34 (9)	C3—C2—H2	121.0
O3—Cu1—Cl2	165.23 (8)	N2—C8—C9$^{\text{ii}}$	111.4 (3)
N1—Cu1—Cl2	95.35 (7)	N2—C8—H27A	109.4
O3—Cu1—Cl1	89.63 (6)	C9$^{\text{ii}}$—C8—H27A	109.4
N1—Cu1—Cl1	170.22 (7)	N2—C8—H27B	109.4
Cl2—Cu1—Cl1	94.33 (3)	C9$^{\text{ii}}$—C8—H27B	109.4
C6—O3—Cu1	116.83 (18)	H27A—C8—H27B	108.0
C5—N1—C1	119.5 (2)	O2—C7—O1	124.8 (3)
C5—N1—Cu1	127.7 (2)	O2—C7—C3	122.5 (3)
C1—N1—Cu1	112.59 (18)	O1—C7—C3	112.7 (3)
C7—O1—H3	109.5	C3—C4—C5	118.7 (3)
O4—C6—O3	124.7 (3)	C3—C4—H12	120.6
O4—C6—C1	120.5 (3)	C5—C4—H12	120.6
O3—C6—C1	114.8 (2)	N1—C5—C4	122.1 (3)
C8—N2—C9	112.0 (2)	N1—C5—H13	118.9
C8—N2—H2A	109.2	C4—C5—H13	118.9
C9—N2—H2A	109.2	C4—C3—C2	119.4 (3)
C8—N2—H2B	109.2	C4—C3—C7	118.0 (3)

C9—N2—H2B	109.2	C2—C3—C7	122.6 (3)
H2A—N2—H2B	107.9	N2—C9—C8^{ii}	110.8 (3)
N1—C1—C2	122.2 (3)	N2—C9—H26A	109.5
N1—C1—C6	113.9 (3)	C8^{ii}—C9—H26A	109.5
C2—C1—C6	123.9 (3)	N2—C9—H26B	109.5
C1—C2—C3	118.0 (3)	C8^{ii}—C9—H26B	109.5
C1—C2—H2	121.0	H26A—C9—H26B	108.1

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H3···O4^{iii}	0.82	1.79	2.603 (3)	171
N2—H2*A*···Cl1^{iv}	0.89	2.78	3.562 (3)	147
N2—H2*A*···O3^{iv}	0.89	2.22	2.861 (3)	129
N2—H2*B*···Cl1^{v}	0.89	2.69	3.414 (3)	139
N2—H2*B*···Cl2^{v}	0.89	2.69	3.360 (3)	133
C2—H2···O2^{vi}	0.93	2.49	3.402 (4)	169
C4—H12···O2^{vii}	0.93	2.56	3.362 (4)	145
C5—H13···Cl2	0.93	2.71	3.269 (3)	119
C8—H27*A*···Cl1^{viii}	0.97	2.72	3.561 (3)	146
C8—H27*B*···Cl2^{ix}	0.97	2.81	3.599 (3)	139
C9—H26*A*···O2^{x}	0.97	2.56	3.509 (4)	165
C9—H26*B*···Cl1^{viii}	0.97	2.93	3.713 (3)	139
C9—H26*B*···Cl2^{v}	0.97	2.93	3.491 (4)	118

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