



Bis(imidazo[1,2-*a*]pyridin-1-ium) tetrachlorido-cuprate(II) dihydrate

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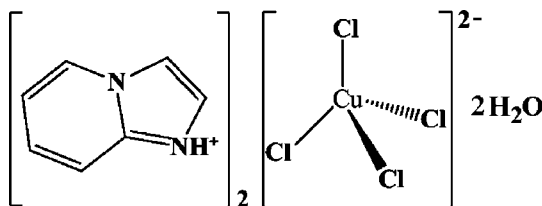
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In the title salt, $(C_7H_7N_2)_2[CuCl_4] \cdot 2H_2O$, the Cu^{2+} cation is coordinated by four Cl atoms and adopts a distorted tetrahedral geometry. Two molecules of imidazo[1,2-*a*]pyridine are protonated ensuring electrical neutrality. $O-H \cdots Cl$ and $N-H \cdots O$ hydrogen bonds link the organic and the inorganic moieties, leading to a self-organized hydrated hybrid structure.

1. Chemical context

Copper halides have applications in biology as antifungal and anticancer agents (Creaven *et al.*, 2010; Santini *et al.*, 2014) and are also good precursors for photovoltaic cells because of their optoelectronic and magnetic properties (Levitsky *et al.*, 2004; Ahmadi *et al.*, 2013; Al-Far & Ali, 2009). For this reason, we have focused our research on copper-based hybrid materials using diverse organic moieties to balance the halide copper inorganic anions. We report in this paper the synthesis and structure determination using single crystal X-ray diffraction data of a tetrahedral tetrachloridocuprate(II) anion with imidazo[1,2-*a*]pyridin-1-ium organic cations and two lattice water molecules.



2. Structural commentary

The structural unit (Fig. 1) of the title compound comprises one $[CuCl_4]^{2-}$ anion, two organic imidazo[1,2-*a*]pyridine ligands and two water molecules.

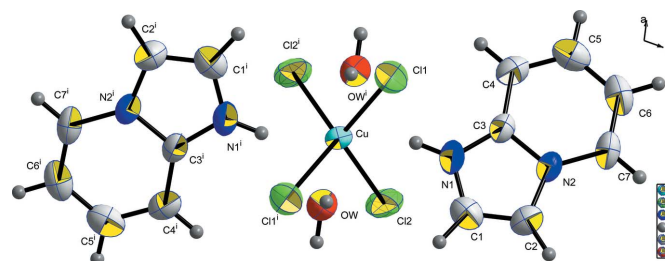
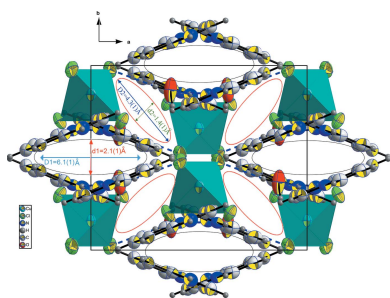


Figure 1
ORTEP-style plot of the structural unit with displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.]

Table 1
 Selected geometric parameters (Å, °).

Cu—Cl2	2.2100 (11)	Cu—Cl1	2.2499 (13)
Cl2—Cu—Cl2 ⁱ	105.26 (7)	Cl2—Cu—Cl1	121.58 (4)
Cl2—Cu—Cl1 ⁱ	102.86 (5)	Cl1 ⁱ —Cu—Cl1	104.12 (7)

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

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

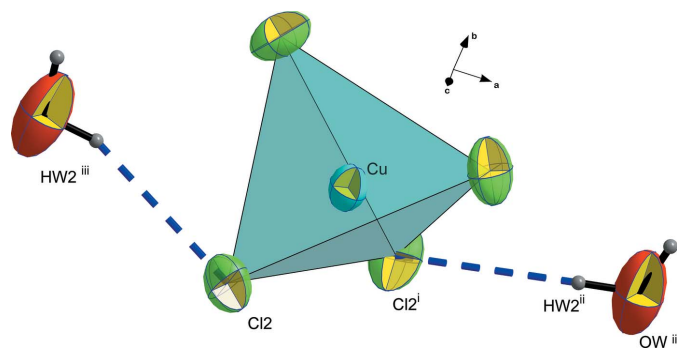
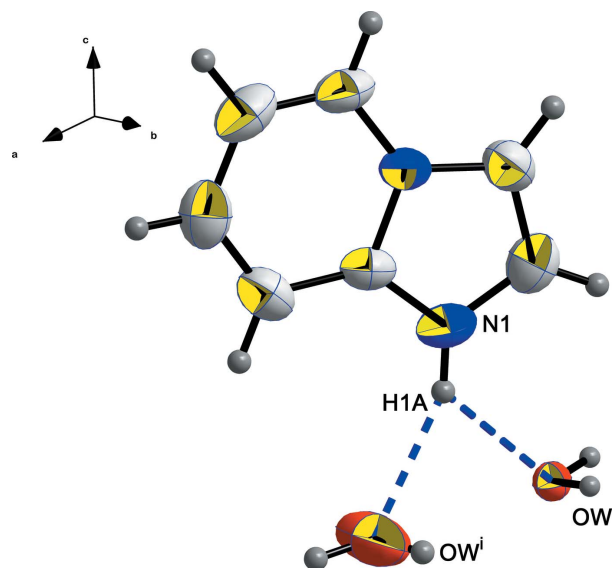
<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1A···OW	0.86	2.50	3.0723	125
N1—H1A···OW ⁱ	0.86	2.08	2.872	152 (1)
OW—HW2···Cl2 ⁱⁱ	0.85	2.61 (1)	3.401	157 (1)

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

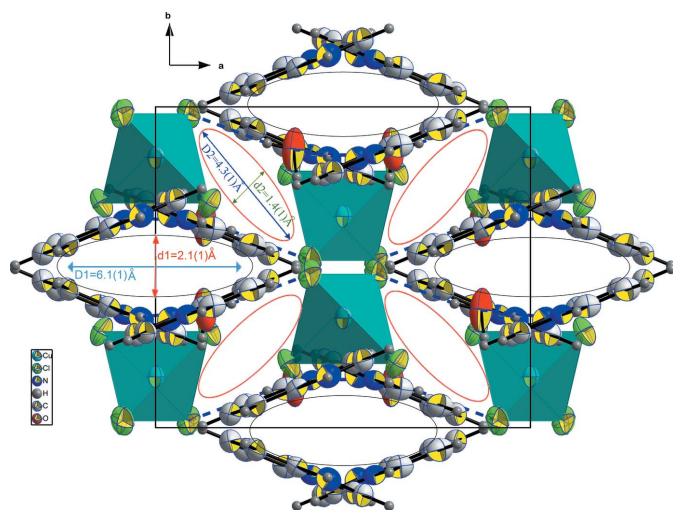
When coordinated by halide anions, copper can adopt several coordination geometries including tetrahedral, square-pyramidal, square-planar and square-bipyramidal (Bhattacharya *et al.*, 2004; Yuan *et al.*, 2004). A four-coordinate geometry is generally intermediate between square-planar and regular-tetrahedral, as reported by Al-Far & Ali (2009). In our case and according to the angular values of the copper–chlorine bonds, summarized in Table 1, the tetrahedral copper coordination seems to be slightly distorted. These distortions are a consequence of the lower molecular symmetry.

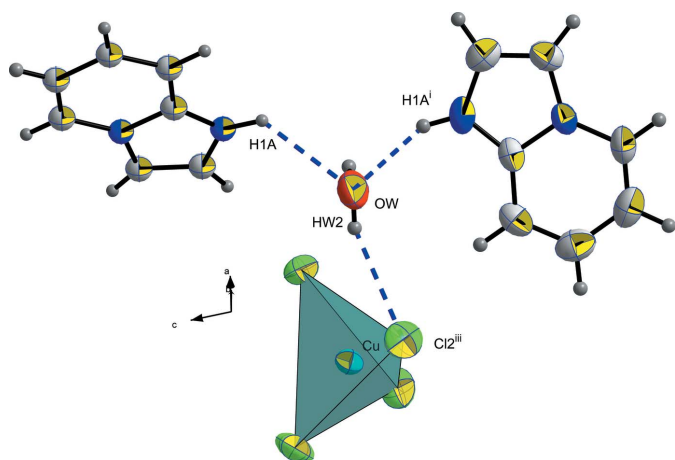
The $(C_7H_7N_2)^+$ cation adopts a quite planar conformation, as characterized by its low r.m.s deviation of 0.0064 Å. The maximum deviations are 0.010 (3) and -0.012 (2) Å for atoms C1 and N2, respectively.

The two water molecules are located approximately in a common plane defined by the organic cations, directing their hydrogen atoms towards the anionic group $[CuCl_4]^{2-}$ and leaving the oxygen free-electron pairs available for a hydrogen-bonding interaction with the protonated nitrogen site of the imidazo[1,2-*a*]pyridinium cation. In the anionic subnetwork, every $[CuCl_4]^{2-}$ anion is linked to two water molecules by hydrogen bonds *via* the Cl2 vertices, as shown in Fig. 2.


Figure 2
 The $[CuCl_4]^{2-}$ environment with hydrogen bonds shown as blue dashed lines. Displacement ellipsoids are displayed at the 50% probability level. [Symmetry codes: (i) $1 - x, y, \frac{1}{2} - z$; (ii) $\frac{1}{2} + x, \frac{1}{2} + y, z$; (iii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

Figure 3
 The environment around the $(C_7H_7N_2)^+$ cation showing the interactions with water molecules through N1—H1A···OW and N1—H1A···OWⁱ interactions. Displacement ellipsoids are displayed at the 50% probability level. [Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.]

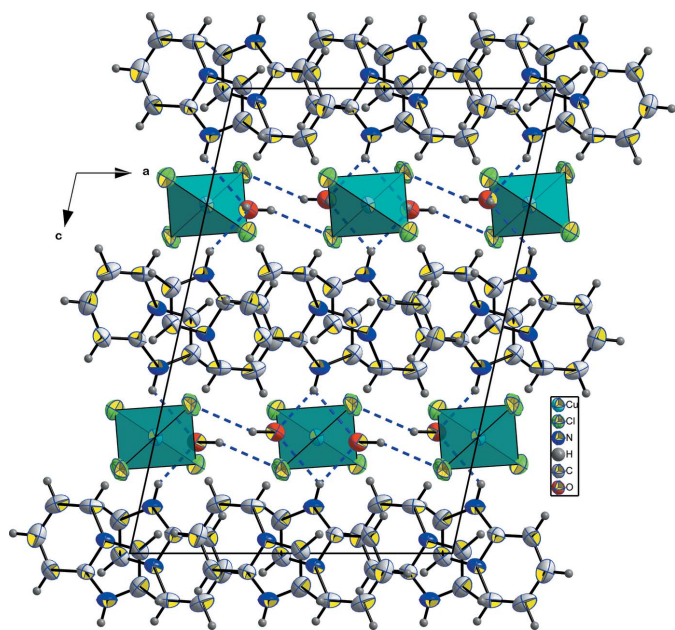
In spite of the single protonation of the organic molecule on the aromatic nitrogen site, every cation is linked to two water molecules through bifurcated hydrogen-bonding interactions along [010], as shown in Fig. 3. The organic cations are organized along (010), forming sheets parallel to the *ab* plane. A projection of the structural packing along the *c* axis, Fig. 4, reveals alternating empty elliptical channels delimited by the organic cations and inorganic tetrahedra. The long and short dimensions of the elliptical sections are estimated to be, respectively, 6.1 (1) and 2.1 (1) Å for the largest ones and 4.3 (1) and 1.4 (1) Å for the narrowest. These voids are able to lodge several small solvent molecules.


Figure 4
 Crystal packing along the *c* axis showing empty tunnels able to lodge small organic solvent molecules. Displacement ellipsoids are displayed at the 50% probability level.


Figure 5

The environment around the water molecule. Hydrogen bonds are indicated by blue dashed lines. Displacement ellipsoids are displayed at the 50% probability level. [Symmetry codes: (i) $1 - x, y, \frac{1}{2} - z$; (iii) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$.]

The water molecules play a crucial role in the crystal-packing cohesion. Every water molecule is linked to one $[\text{CuCl}_4]^{2-}$ tetrahedron through $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2) and to two organic molecules through $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, as shown in Fig. 5. The expected structural self-organization generally present in hybrid inorganic-organic compounds can also be found in the structure of the title salt. The alternating stacking of organic and inorganic sheets observed along the c axis (Fig. 6) could possibly lead to luminescence properties.


Figure 6

View of the packing showing the alternating stacking of the organic and inorganic layers connected through hydrogen bonds. The face-to-face $\pi-\pi$ stacking between parallel organic molecules is noteworthy with a centroid-centroid distance of 3.968 (3) Å. Displacement ellipsoids are displayed at the 50% probability level. [Symmetry code: (iii) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$.]

Table 3

Experimental details.

Crystal data	$(\text{C}_7\text{H}_7\text{N}_2)_2[\text{CuCl}_4]\cdot 2\text{H}_2\text{O}$
Chemical formula	479.66
M_r	Monoclinic, $C2/c$
Crystal system, space group	298
Temperature (K)	a, b, c (Å)
a, b, c (Å)	11.747 (8), 9.793 (2), 17.339 (4)
β (°)	102.48 (5)
V (Å ³)	1947.7 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.69
Crystal size (mm)	0.45 × 0.15 × 0.1
Data collection	
Diffractometer	Enraf-Nonius CAD-4
Absorption correction	ψ scan (North <i>et al.</i> , 1968).
$T_{\text{min}}, T_{\text{max}}$	0.746, 0.845
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3358, 2127, 1796
R_{int}	0.042
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.038, 0.108, 1.04
No. of reflections	2127
No. of parameters	120
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.78, -0.49

Computer programs: *CAD-4 EXPRESS* (Enraf-Nonius, 1994), *XCAD4* (Harms & Wocadlo, 1995), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006) and *pubCIF* (Westrip, 2010).

3. Supramolecular features

The lowering of the symmetry of the copper coordination could also be due to halide-halide and intra- and intermolecular hydrogen-bonding interactions; these interactions are closely related to the shape and the size of the counter-cations (Bouacida *et al.*, 2013; Parent *et al.*, 2007; Haddad *et al.*, 2006; Marzotto *et al.*, 2001; Choi *et al.*, 2002; Awwadi *et al.*, 2007). Non-covalent interactions such as hydrogen-bonding interactions and $\pi-\pi$ stacking interactions represent the most important linkers in this kind of material. Moreover, these interactions are able to delimit not only the architecture, but also impact on the properties of metal-halide materials. The organic cations are linked to the water molecule through $\text{N1}-\text{H1A}\cdots\text{OW}$ hydrogen bonds (Table 2) and are connected through face-to-face $\pi-\pi$ stacking [$\text{Cg1}\cdots\text{Cg2}(\frac{3}{2} - x, \frac{1}{2} - y, 1 - z) = 3.968$ (3) Å where Cg1 and Cg2 are the centroids of the N1/N3/C1-C3 and N2/C3-C7 rings, respectively]. The crystal packing can be described by alternating stacks of anions and cationic chains with the organic layers arranged parallel to the anionic stacks.

4. Database survey

Imidazo[1,2-*a*]-pyridyn-1-ium cations and several substituted forms have 53 entries in the Cambridge Structural Database (Groom *et al.*, 2016) without any hybrid compounds amongst

them. To the best of our knowledge, this work is the first chemical and crystallographic identification of tetrachloridocuprate(II) combined with imidazo[1,2-*a*]-pyridyn-1-ium.

5. Synthesis and crystallization

The title salt was prepared by the reaction of imidazo[1,2-*a*]-pyridine and $\text{Cu}(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ (molar ratio 1:1) in an equal volume of water and ethanol (10 ml) mixed with 2 ml of hydrochloric acid (37%). The solution was stirred for 1 h at 333 K. Prismatic yellow crystals suitable for X-ray diffraction were grown in one week by slow evaporation at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically and treated as riding on the parent atom with $\text{C}-\text{H} = 0.93 \text{ \AA}$ and $\text{N}-\text{H} = 0.86 \text{ \AA}$. For HW1 and HW2, the restraints DFIX and DANG were used to stabilize the water molecule.

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supporting information

Acta Cryst. (2017). E73, 196-199 [https://doi.org/10.1107/S2056989017000482]

Bis(imidazo[1,2-a]pyridin-1-ium) tetrachloridocuprate(II) dihydrate

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Computing details

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis(imidazo[1,2-a]pyridin-1-ium) tetrachloridocuprate(II) dihydrate

Crystal data

$(C_7H_7N_2)_2[CuCl_4] \cdot 2H_2O$

$M_r = 479.66$

Monoclinic, *C2/c*

$a = 11.747$ (8) Å

$b = 9.793$ (2) Å

$c = 17.339$ (4) Å

$\beta = 102.48$ (5)°

$V = 1947.7$ (15) Å³

$Z = 4$

$F(000) = 972$

$D_x = 1.636$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 2-27^\circ$

$\mu = 1.69$ mm⁻¹

$T = 298$ K

Prism, yellow

$0.45 \times 0.15 \times 0.1$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube
non-profiled $\omega/2\tau$ scans

Absorption correction: ψ scan
(North *et al.*, 1968).

$T_{\min} = 0.746$, $T_{\max} = 0.845$

3358 measured reflections

2127 independent reflections

1796 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -14 \rightarrow 4$

$k = -1 \rightarrow 12$

$l = -22 \rightarrow 22$

2 standard reflections every 120 min

intensity decay: 32%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.108$

$S = 1.04$

2127 reflections

120 parameters

3 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 3.2027P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.78$ e Å⁻³

$\Delta\rho_{\min} = -0.49$ 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu	0.5000	0.65843 (5)	0.2500	0.03734 (16)
Cl1	0.64409 (8)	0.79968 (10)	0.30835 (5)	0.0654 (3)
Cl2	0.41162 (7)	0.52147 (11)	0.31978 (6)	0.0691 (3)
N1	0.5383 (2)	0.1611 (3)	0.39993 (14)	0.0503 (6)
H1A	0.5411	0.1555	0.3509	0.060*
N2	0.5837 (2)	0.1477 (2)	0.52756 (13)	0.0407 (5)
C1	0.4463 (3)	0.2105 (4)	0.4280 (2)	0.0564 (8)
H1	0.3770	0.2439	0.3973	0.068*
C2	0.4724 (3)	0.2029 (3)	0.50690 (19)	0.0508 (7)
H2	0.4254	0.2294	0.5411	0.061*
C3	0.6232 (2)	0.1228 (3)	0.46046 (15)	0.0411 (6)
C4	0.7339 (3)	0.0682 (3)	0.4645 (2)	0.0522 (7)
H4	0.7615	0.0503	0.4191	0.063*
C5	0.8004 (3)	0.0420 (4)	0.5383 (2)	0.0608 (8)
H5	0.8747	0.0056	0.5433	0.073*
C6	0.7581 (3)	0.0691 (4)	0.6061 (2)	0.0614 (9)
H6	0.8047	0.0507	0.6556	0.074*
C7	0.6512 (3)	0.1214 (3)	0.60080 (17)	0.0528 (7)
H7	0.6234	0.1394	0.6461	0.063*
OW	0.3680 (2)	0.1331 (5)	0.23911 (17)	0.0959 (12)
HW1	0.376 (5)	0.2194 (15)	0.244 (5)	0.144*
HW2	0.2977 (19)	0.114 (5)	0.238 (4)	0.144*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0303 (2)	0.0469 (3)	0.0372 (2)	0.000	0.01252 (17)	0.000
Cl1	0.0549 (5)	0.0787 (6)	0.0612 (5)	-0.0256 (4)	0.0092 (4)	-0.0132 (4)
Cl2	0.0553 (5)	0.0861 (6)	0.0731 (5)	-0.0074 (4)	0.0300 (4)	0.0268 (5)
N1	0.0616 (15)	0.0559 (15)	0.0321 (11)	-0.0059 (12)	0.0070 (11)	0.0009 (10)
N2	0.0518 (13)	0.0387 (12)	0.0339 (10)	-0.0029 (10)	0.0143 (10)	0.0000 (9)
C1	0.0509 (17)	0.0544 (18)	0.0594 (19)	-0.0002 (14)	0.0022 (14)	0.0033 (15)
C2	0.0522 (17)	0.0501 (16)	0.0544 (17)	0.0015 (13)	0.0208 (14)	0.0002 (14)
C3	0.0502 (15)	0.0410 (13)	0.0337 (12)	-0.0089 (11)	0.0128 (11)	-0.0028 (11)
C4	0.0546 (17)	0.0505 (16)	0.0570 (17)	-0.0064 (13)	0.0239 (14)	-0.0077 (14)
C5	0.0485 (17)	0.0515 (18)	0.079 (2)	-0.0010 (14)	0.0060 (16)	-0.0004 (17)

C6	0.074 (2)	0.0547 (18)	0.0467 (17)	-0.0044 (16)	-0.0062 (16)	0.0051 (15)
C7	0.074 (2)	0.0523 (17)	0.0312 (13)	-0.0027 (15)	0.0085 (13)	0.0015 (12)
OW	0.0537 (15)	0.186 (4)	0.0483 (14)	-0.0107 (19)	0.0127 (12)	0.010 (2)

Geometric parameters (Å, °)

Cu—Cl2	2.2100 (11)	C2—H2	0.9300
Cu—Cl2 ⁱ	2.2100 (11)	C3—C4	1.394 (4)
Cu—Cl1 ⁱ	2.2499 (13)	C4—C5	1.372 (5)
Cu—Cl1	2.2499 (13)	C4—H4	0.9300
N1—C3	1.336 (4)	C5—C6	1.397 (6)
N1—C1	1.366 (5)	C5—H5	0.9300
N1—H1A	0.8600	C6—C7	1.340 (5)
N2—C3	1.364 (3)	C6—H6	0.9300
N2—C7	1.369 (4)	C7—H7	0.9300
N2—C2	1.388 (4)	OW—HW1	0.854 (10)
C1—C2	1.338 (5)	OW—HW2	0.845 (10)
C1—H1	0.9300		
Cl2—Cu—Cl2 ⁱ	105.26 (7)	N2—C2—H2	126.8
Cl2—Cu—Cl1 ⁱ	102.86 (5)	N1—C3—N2	106.6 (3)
Cl2 ⁱ —Cu—Cl1 ⁱ	121.58 (4)	N1—C3—C4	132.6 (3)
Cl2—Cu—Cl1	121.58 (4)	N2—C3—C4	120.7 (3)
Cl2 ⁱ —Cu—Cl1	102.86 (5)	C5—C4—C3	117.1 (3)
Cl1 ⁱ —Cu—Cl1	104.12 (7)	C5—C4—H4	121.5
C3—N1—C1	109.5 (3)	C3—C4—H4	121.5
C3—N1—H1A	125.3	C4—C5—C6	121.0 (3)
C1—N1—H1A	125.3	C4—C5—H5	119.5
C3—N2—C7	121.5 (3)	C6—C5—H5	119.5
C3—N2—C2	108.9 (2)	C7—C6—C5	120.8 (3)
C7—N2—C2	129.6 (3)	C7—C6—H6	119.6
C2—C1—N1	108.7 (3)	C5—C6—H6	119.6
C2—C1—H1	125.7	C6—C7—N2	118.9 (3)
N1—C1—H1	125.7	C6—C7—H7	120.6
C1—C2—N2	106.3 (3)	N2—C7—H7	120.6
C1—C2—H2	126.8	HW1—OW—HW2	108 (3)

Symmetry code: (i) $-x+1, y, -z+1/2$.*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots OW	0.86	2.50	3.0723	125
N1—H1A \cdots OW ⁱ	0.86	2.08	2.872	152 (1)
OW—HW2 \cdots Cl2 ⁱⁱ	0.85	2.61 (1)	3.401	157 (1)

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