Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# 2-Oxo-1,2-dihydropyrimidin-3-ium di-$\mu$-chlorido-bis{dichloridobis[pyrimidin-2(1*H*)-one-$\kappa N^3$]cuprate(II)} dihydrate

**Mukhtar A. Kurawa, Christopher J. Adams and A. Guy Orpen***

School of Chemistry, University of Bristol, Bristol BS8 1TS, England
Correspondence e-mail: guy.orpen@bristol.ac.uk

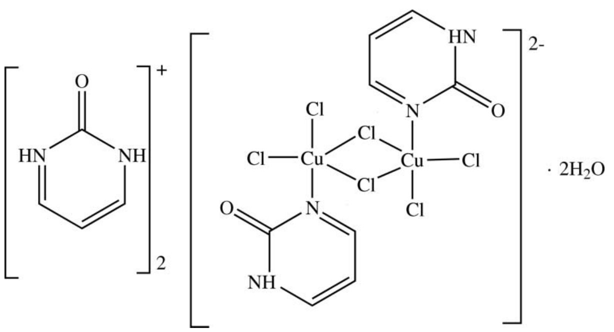
Received 9 June 2008; accepted 10 June 2008

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; *R* factor = 0.024; *wR* factor = 0.070; data-to-parameter ratio = 21.7.

The asymmetric unit of the title compound, $(C_4H_5N_2O)_2[Cu_2Cl_6(C_4H_4N_2O)_2]\cdot 2H_2O$, consists of one cation, one half of a centrosymmetric dianion and one water molecule. The centrosymmetric dianion formed by dimerization in the crystal structure has neutral pyrimidin-2-one ligands coordinated to each copper(II) centre through Cu—N bonds. The Cu atoms each have a distorted trigonal bipyramidal geometry, with the N atom of the pyrimidin-2-one ligand in an axial position, and dimerize by sharing two equatorial Cl atoms. N—H···Cl, O—H···Cl and N—H···O hydrogen bonds connect the anions, cations and water molecules, forming a three-dimensional network.

## Related literature

The anion has an essentially similar coordination environment to that of the related compound $[\{(C_5H_5N)NH_2\}CuCl_3]_2$ which has 3-aminopyridinium cations (Blanchette & Willett, 1988) as the nitrogen donors and is thus neutral, while the crystal structure of the cation was described by Furberg & Aas (1975) as its chloride salt.



## Experimental

### *Crystal data*

$(C_4H_5N_2O)_2[Cu_2Cl_6(C_4H_4N_2O)_2]\cdot$-$2H_2O$
$M_r$ = 762.22
Triclinic, $P\overline{1}$
$a$ = 7.5924 (4) Å
$b$ = 8.6401 (3) Å
$c$ = 10.6349 (4) Å
$\alpha$ = 96.032 (3)°
$\beta$ = 100.508 (4)°
$\gamma$ = 102.035 (4)°
$V$ = 663.39 (5) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 2.26 mm$^{-1}$
$T$ = 100 (2) K
0.41 × 0.18 × 0.15 mm

### *Data collection*

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.433, $T_{max}$ = 0.71
14528 measured reflections
3902 independent reflections
3269 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.069
$S$ = 1.12
3902 reflections
180 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.57 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.9989 (12) | Cu1—Cl2$^i$ | 2.3942 (4) |
| Cu1—Cl3 | 2.2809 (4) | Cu1—Cl2 | 2.6093 (4) |
| Cu1—Cl1 | 2.2830 (4) | | |

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

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*B*···Cl1$^{ii}$ | 0.86 | 2.56 | 3.4143 (14) | 171 |
| N3—H3*A*···O3$^{iii}$ | 0.86 | 1.86 | 2.7099 (18) | 168 |
| N4—H2*A*···Cl2$^{iv}$ | 0.86 | 2.30 | 3.1336 (14) | 165 |
| O3—H1···Cl1$^{v}$ | 0.815 (16) | 2.428 (17) | 3.2258 (13) | 166 (2) |
| O3—H2···Cl3$^{vi}$ | 0.844 (17) | 2.454 (18) | 3.2653 (13) | 162 (2) |

Symmetry codes: (ii) $x, y-1, z$; (iii) $x, y+1, z$; (iv) $x, y, z-1$; (v) $-x+1, -y+1, -z+1$; (vi) $x+1, y, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *SHELXTL*).

MAK thanks Bayero University, Kano, Nigeria, for funding. Oxford Diffraction Ltd are thanked for the loan of an Oxford Gemini R Ultra diffractometer to the University of Bristol.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2250).

## References

Blanchette, J. T. & Willett, R. D. (1988). *Inorg. Chem.* **27**, 843–849.

Furberg, S. & Aas, J. B. (1975). *Acta Chem. Scand.* **A29**, 713–716.

Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.

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

*Acta Cryst.* (2008). E**64**, m924–m925 Kurawa *et al.* • $(C_4H_5N_2O)_2[Cu_2Cl_6(C_4H_4N_2O)_2]\cdot 2H_2O$ **m925**

# supplementary materials

*Acta Cryst.* (2008). E**64**, m924-m925 [ **doi:10.1107/S1600536808017455** ]

# 2-Oxo-1,2-dihydropyrimidin-3-ium di-$\mu$-chlorido-bis{dichloridobis[pyrimidin-2(1*H*)-one-$\kappa N^3$]cuprate(II)} dihydrate

**M. A. Kurawa, C. J. Adams and A. G. Orpen**

## Comment

N—H···Cl interactions have been extensively used in crystal engineering to design and synthesize materials with desired structures. We sought to further utilize these interactions by reacting 2-hydroxypyrimidine hydrochloride and copper(II) chloride in a 2:1 ratio with the aim of synthesizing $[C_4H_5N_2O]_2[CuCl_4]$. However, the title compound **I** was obtained, which crystallizes in the triclinic system with the $P\overline{1}$ space group. The copper coordination centres are similar to those described by Blanchette and Willett (1988) in $[\{(C_5H_5N)NH_2\}CuCl_3]_2$. The $H_2O$ molecules and the $[C_4H_5N_2O]^+$ cations (having both N atoms protonated and the O atoms atom deprotonated) are packed between the anions along the *c*-axis, the water forming O—H···Cl bridges between the anions while the cations form N—H···Cl and N—H···O bonds with the anions and water molecules respectively (Fig. 2).

For related literature, see Blanchette & Willett (1988) and Furberg & Aas (1975).

## Experimental

Copper(II) chloride dihydrate and 2-hydroxypyrimidine hydrochloride in a 1:2 molar ratio were dissolved in concentrated hydrochloric acid solution. The solution was left to evaporate slowly at room temperature and resulted in the formation of green crystals after a few days.

## Refinement

H atoms bonded to O atoms were located in the difference map and refined with distance restraints of O—H = 0.84 (2) Å with $U_{iso}(H) = 1.2U_{eq}(O)$. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and N—H = 0.86 Å, with $U_{iso}(H)$ = 1.2 times $U_{eq}$(C, N).

## Figures

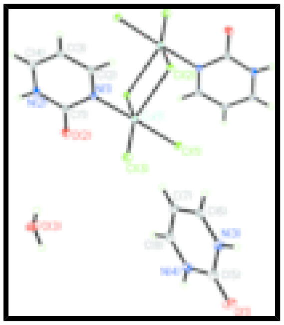


Fig. 1. The molecular structure of **I** showing one dimeric dianion, one cation and a molecule of water of crystallization, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

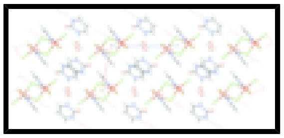


Fig. 2. Packing of **I** in the *ac* plane, with O—H···Cl bridges between the water molecules and the dianions, N—H···O hydrogen bonds between cations and water molecules, and N—H···Cl hydrogen bonds between the anions and cations.

### 2-Oxo-1,2-dihydropyrimidin-3-ium di-μ-chlorido-bis{dichloridobis[pyrimidin-2(1H)-one-κN$^3$]cuprate(II)} dihydrate

*Crystal data*

| | |
|---|---|
| $(C_4H_5N_2O)_2[Cu_2Cl_6(C_4H_4N_2O)_2]\cdot 2H_2O$ | $Z = 1$ |
| $M_r = 762.22$ | $F_{000} = 382$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.908$ Mg m$^{-3}$ |
| $a = 7.5924$ (4) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 8.6401$ (3) Å | Cell parameters from 10481 reflections |
| $c = 10.6349$ (4) Å | $\theta = 2.4$–$30.0$° |
| $\alpha = 96.032$ (3)° | $\mu = 2.26$ mm$^{-1}$ |
| $\beta = 100.508$ (4)° | $T = 100$ (2) K |
| $\gamma = 102.035$ (4)° | Block, green |
| $V = 663.39$ (5) Å$^3$ | 0.41 × 0.18 × 0.16 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini-R Ultra diffractometer | 3902 independent reflections |
| Radiation source: fine-focus sealed tube | 3269 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 100(2)$ K | $\theta_{max} = 30.1$° |
| ω (1° width) scans | $\theta_{min} = 2.4$° |
| Absorption correction: multi-scan<br>(CrysAlis RED; Oxford Diffraction, 2007) | $h = -10\rightarrow 10$ |
| $T_{min} = 0.433$, $T_{max} = 0.71$ | $k = -12\rightarrow 12$ |
| 14528 measured reflections | $l = -15\rightarrow 15$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.069$ | $w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.0753P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.12$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 3902 reflections | $\Delta\rho_{max} = 0.49$ e Å$^{-3}$ |
| 180 parameters | $\Delta\rho_{min} = -0.57$ e Å$^{-3}$ |

| | |
|---|---|
| 2 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Special details*

**Experimental**. CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.32.5 (release 08-05-2007 CrysAlis171 .NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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. 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.07237 (3) | 0.45037 (2) | 0.848449 (17) | 0.01007 (6) |
| Cl1 | −0.06435 (5) | 0.63425 (4) | 0.75599 (3) | 0.01291 (8) |
| Cl2 | 0.19396 (5) | 0.64570 (4) | 1.06611 (3) | 0.01065 (8) |
| Cl3 | 0.26769 (6) | 0.45986 (5) | 0.70847 (4) | 0.01557 (9) |
| N1 | 0.18231 (18) | 0.28152 (15) | 0.92487 (12) | 0.0099 (2) |
| N2 | 0.15847 (19) | 0.00585 (15) | 0.91842 (13) | 0.0122 (3) |
| H2B | 0.1020 | −0.0912 | 0.8865 | 0.015* |
| N3 | 0.69462 (19) | 0.93935 (16) | 0.46681 (12) | 0.0124 (3) |
| H3A | 0.7819 | 1.0237 | 0.4760 | 0.015* |
| N4 | 0.43187 (19) | 0.76169 (16) | 0.34665 (13) | 0.0137 (3) |
| H2A | 0.3488 | 0.7298 | 0.2768 | 0.016* |
| O1 | 0.58355 (18) | 0.96484 (15) | 0.25699 (12) | 0.0204 (3) |
| O2 | −0.02211 (17) | 0.10178 (14) | 0.76366 (11) | 0.0176 (2) |
| O3 | 0.93114 (18) | 0.22792 (15) | 0.49005 (12) | 0.0198 (3) |
| C1 | 0.0983 (2) | 0.12810 (17) | 0.86166 (15) | 0.0116 (3) |
| C2 | 0.3215 (2) | 0.30666 (18) | 1.02403 (14) | 0.0119 (3) |
| H2C | 0.3773 | 0.4116 | 1.0619 | 0.014* |
| C3 | 0.3900 (2) | 0.18275 (18) | 1.07546 (15) | 0.0132 (3) |
| H3B | 0.4917 | 0.2036 | 1.1436 | 0.016* |
| C4 | 0.3004 (2) | 0.03050 (18) | 1.02078 (15) | 0.0129 (3) |
| H4A | 0.3368 | −0.0560 | 1.0538 | 0.016* |
| C5 | 0.5717 (2) | 0.89360 (19) | 0.34849 (15) | 0.0135 (3) |
| C6 | 0.6850 (2) | 0.85959 (19) | 0.56744 (15) | 0.0134 (3) |
| H6A | 0.7744 | 0.8941 | 0.6433 | 0.016* |
| C7 | 0.5451 (2) | 0.72742 (19) | 0.56028 (15) | 0.0141 (3) |
| H7A | 0.5372 | 0.6718 | 0.6301 | 0.017* |
| C8 | 0.4167 (2) | 0.68029 (19) | 0.44567 (15) | 0.0139 (3) |
| H8A | 0.3194 | 0.5917 | 0.4373 | 0.017* |

| | | | | |
|---|---|---|---|---|
| H1 | 0.947 (3) | 0.268 (3) | 0.4257 (19) | 0.037 (7)* |
| H2 | 1.024 (3) | 0.267 (3) | 0.551 (2) | 0.044 (8)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.01130 (11) | 0.00927 (9) | 0.00972 (10) | 0.00265 (7) | 0.00141 (7) | 0.00270 (7) |
| Cl1 | 0.01491 (19) | 0.01236 (16) | 0.01204 (17) | 0.00437 (13) | 0.00135 (14) | 0.00458 (12) |
| Cl2 | 0.01105 (17) | 0.00891 (15) | 0.01027 (16) | 0.00021 (13) | 0.00046 (13) | 0.00112 (12) |
| Cl3 | 0.01575 (19) | 0.01618 (18) | 0.01615 (18) | 0.00296 (14) | 0.00692 (14) | 0.00377 (14) |
| N1 | 0.0118 (6) | 0.0074 (5) | 0.0097 (6) | 0.0012 (5) | 0.0015 (5) | 0.0009 (4) |
| N2 | 0.0136 (7) | 0.0069 (5) | 0.0160 (6) | 0.0012 (5) | 0.0042 (5) | 0.0008 (5) |
| N3 | 0.0102 (6) | 0.0135 (6) | 0.0123 (6) | 0.0010 (5) | 0.0007 (5) | 0.0024 (5) |
| N4 | 0.0115 (6) | 0.0165 (6) | 0.0101 (6) | 0.0018 (5) | −0.0021 (5) | −0.0012 (5) |
| O1 | 0.0218 (7) | 0.0265 (6) | 0.0160 (6) | 0.0084 (5) | 0.0052 (5) | 0.0100 (5) |
| O2 | 0.0184 (6) | 0.0142 (5) | 0.0158 (5) | 0.0017 (5) | −0.0033 (5) | −0.0013 (4) |
| O3 | 0.0198 (7) | 0.0203 (6) | 0.0143 (6) | −0.0049 (5) | 0.0001 (5) | 0.0058 (5) |
| C1 | 0.0126 (7) | 0.0089 (6) | 0.0133 (7) | 0.0014 (5) | 0.0040 (6) | 0.0013 (5) |
| C2 | 0.0122 (7) | 0.0106 (7) | 0.0122 (7) | 0.0019 (6) | 0.0025 (6) | 0.0010 (5) |
| C3 | 0.0140 (8) | 0.0136 (7) | 0.0125 (7) | 0.0049 (6) | 0.0019 (6) | 0.0025 (5) |
| C4 | 0.0149 (8) | 0.0121 (7) | 0.0149 (7) | 0.0058 (6) | 0.0059 (6) | 0.0056 (6) |
| C5 | 0.0114 (8) | 0.0157 (7) | 0.0141 (7) | 0.0052 (6) | 0.0022 (6) | 0.0023 (6) |
| C6 | 0.0139 (8) | 0.0137 (7) | 0.0115 (7) | 0.0041 (6) | −0.0005 (6) | 0.0009 (5) |
| C7 | 0.0160 (8) | 0.0139 (7) | 0.0119 (7) | 0.0028 (6) | 0.0022 (6) | 0.0030 (5) |
| C8 | 0.0121 (8) | 0.0128 (7) | 0.0158 (7) | 0.0020 (6) | 0.0030 (6) | −0.0004 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.9989 (12) | N4—H2A | 0.8600 |
| Cu1—Cl3 | 2.2809 (4) | O1—C5 | 1.2119 (19) |
| Cu1—Cl1 | 2.2830 (4) | O2—C1 | 1.221 (2) |
| Cu1—Cl2$^{i}$ | 2.3942 (4) | O3—H1 | 0.815 (16) |
| Cu1—Cl2 | 2.6093 (4) | O3—H2 | 0.844 (17) |
| Cl2—Cu1$^{i}$ | 2.3942 (4) | C2—C3 | 1.403 (2) |
| N1—C2 | 1.314 (2) | C2—H2C | 0.9300 |
| N1—C1 | 1.3854 (19) | C3—C4 | 1.361 (2) |
| N2—C4 | 1.349 (2) | C3—H3B | 0.9300 |
| N2—C1 | 1.3868 (19) | C4—H4A | 0.9300 |
| N2—H2B | 0.8600 | C6—C7 | 1.373 (2) |
| N3—C6 | 1.337 (2) | C6—H6A | 0.9300 |
| N3—C5 | 1.387 (2) | C7—C8 | 1.378 (2) |
| N3—H3A | 0.8600 | C7—H7A | 0.9300 |
| N4—C8 | 1.335 (2) | C8—H8A | 0.9300 |
| N4—C5 | 1.382 (2) | | |
| N1—Cu1—Cl3 | 88.53 (4) | O2—C1—N1 | 122.46 (14) |
| N1—Cu1—Cl1 | 177.38 (4) | O2—C1—N2 | 122.11 (14) |
| Cl3—Cu1—Cl1 | 91.956 (15) | N1—C1—N2 | 115.42 (13) |
| N1—Cu1—Cl2$^{i}$ | 88.05 (4) | N1—C2—C3 | 123.13 (14) |

| | | | |
|---|---|---|---|
| Cl3—Cu1—Cl2$^{i}$ | 157.928 (16) | N1—C2—H2C | 118.4 |
| Cl1—Cu1—Cl2$^{i}$ | 90.538 (15) | C3—C2—H2C | 118.4 |
| N1—Cu1—Cl2 | 91.12 (4) | C4—C3—C2 | 116.78 (15) |
| Cl3—Cu1—Cl2 | 115.984 (15) | C4—C3—H3B | 121.6 |
| Cl1—Cu1—Cl2 | 90.982 (14) | C2—C3—H3B | 121.6 |
| Cl2$^{i}$—Cu1—Cl2 | 85.883 (14) | N2—C4—C3 | 119.63 (14) |
| Cu1$^{i}$—Cl2—Cu1 | 94.117 (14) | N2—C4—H4A | 120.2 |
| C2—N1—C1 | 120.92 (13) | C3—C4—H4A | 120.2 |
| C2—N1—Cu1 | 125.69 (10) | O1—C5—N4 | 123.48 (15) |
| C1—N1—Cu1 | 113.38 (10) | O1—C5—N3 | 123.19 (15) |
| C4—N2—C1 | 123.75 (13) | N4—C5—N3 | 113.30 (13) |
| C4—N2—H2B | 118.1 | N3—C6—C7 | 120.87 (15) |
| C1—N2—H2B | 118.1 | N3—C6—H6A | 119.6 |
| C6—N3—C5 | 123.65 (14) | C7—C6—H6A | 119.6 |
| C6—N3—H3A | 118.2 | C6—C7—C8 | 117.45 (15) |
| C5—N3—H3A | 118.2 | C6—C7—H7A | 121.3 |
| C8—N4—C5 | 124.63 (14) | C8—C7—H7A | 121.3 |
| C8—N4—H2A | 117.7 | N4—C8—C7 | 120.03 (15) |
| C5—N4—H2A | 117.7 | N4—C8—H8A | 120.0 |
| H1—O3—H2 | 109 (2) | C7—C8—H8A | 120.0 |

| | | | |
|---|---|---|---|
| N1—Cu1—Cl2—Cu1$^{i}$ | −87.97 (4) | C4—N2—C1—N1 | −6.1 (2) |
| Cl3—Cu1—Cl2—Cu1$^{i}$ | −176.875 (16) | C1—N1—C2—C3 | −2.4 (2) |
| Cl1—Cu1—Cl2—Cu1$^{i}$ | 90.469 (15) | Cu1—N1—C2—C3 | 178.41 (11) |
| Cl2$^{i}$—Cu1—Cl2—Cu1$^{i}$ | 0.0 | N1—C2—C3—C4 | −2.5 (2) |
| Cl3—Cu1—N1—C2 | 92.08 (13) | C1—N2—C4—C3 | 1.5 (2) |
| Cl2$^{i}$—Cu1—N1—C2 | −109.72 (13) | C2—C3—C4—N2 | 2.9 (2) |
| Cl2—Cu1—N1—C2 | −23.88 (13) | C8—N4—C5—O1 | 179.35 (16) |
| Cl3—Cu1—N1—C1 | −87.19 (10) | C8—N4—C5—N3 | −2.3 (2) |
| Cl2$^{i}$—Cu1—N1—C1 | 71.00 (10) | C6—N3—C5—O1 | −178.50 (16) |
| Cl2—Cu1—N1—C1 | 156.84 (10) | C6—N3—C5—N4 | 3.2 (2) |
| C2—N1—C1—O2 | −174.50 (15) | C5—N3—C6—C7 | −2.4 (2) |
| Cu1—N1—C1—O2 | 4.8 (2) | N3—C6—C7—C8 | 0.4 (2) |
| C2—N1—C1—N2 | 6.4 (2) | C5—N4—C8—C7 | 0.7 (2) |
| Cu1—N1—C1—N2 | −174.26 (10) | C6—C7—C8—N4 | 0.4 (2) |
| C4—N2—C1—O2 | 174.79 (15) | | |

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

### *Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2B···Cl1$^{ii}$ | 0.86 | 2.56 | 3.4143 (14) | 171 |
| N3—H3A···O3$^{iii}$ | 0.86 | 1.86 | 2.7099 (18) | 168 |
| N4—H2A···Cl2$^{iv}$ | 0.86 | 2.30 | 3.1336 (14) | 165 |
| O3—H1···Cl1$^{v}$ | 0.815 (16) | 2.428 (17) | 3.2258 (13) | 166 (2) |
| O3—H2···Cl3$^{vi}$ | 0.844 (17) | 2.454 (18) | 3.2653 (13) | 162 (2) |

Symmetry codes: (ii) *x*, *y*−1, *z*; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*, *z*−1; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*+1, *y*, *z*.

**Fig. 1**

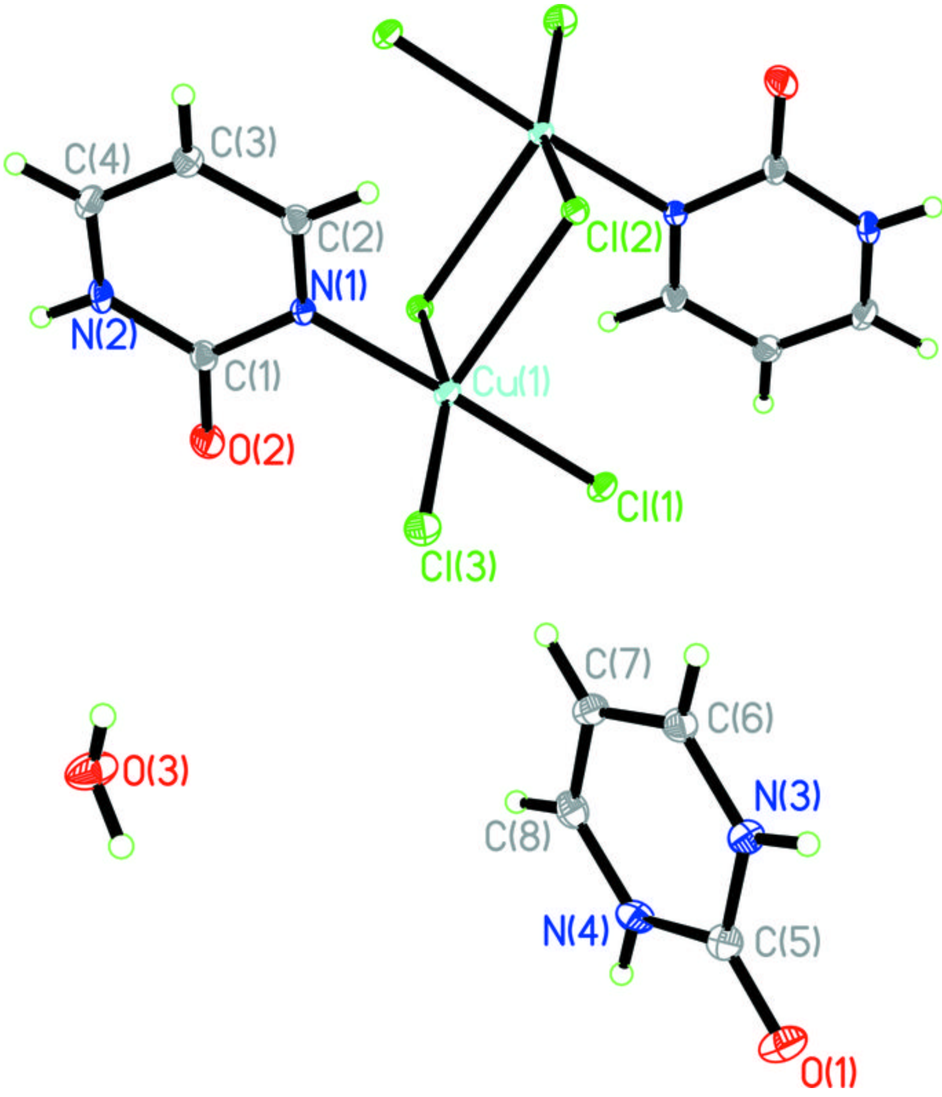


**Fig. 2**