

# { $\mu$ -1,5-Bis[(*E*)-1-(2-pyridyl)ethylidene]-carbonohydrazidato(1-)]bis[chlorido-methanolcopper(II)] perchlorate

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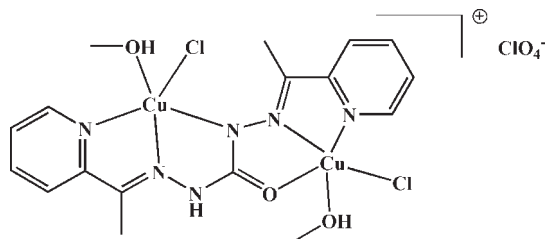
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.142; data-to-parameter ratio = 17.9.

The title dinuclear copper complex,  $[\text{Cu}_2(\text{C}_{15}\text{H}_{15}\text{N}_6\text{O})\text{Cl}_2(\text{CH}_3\text{OH})_2]\text{ClO}_4$ , was prepared by the reaction of copper(II) chloride with bis[1-(2-pyridyl)ethylidene]carbonohydrazide in the presence of sodium perchlorate in a methanol solution. It features a mono-deprotonated bis-tridentate ligand, which coordinates to two independent  $\text{Cu}^{\text{II}}$  ions, one of which is coordinated by pyridyl N, hydrazyl N and carbonyl O atoms. The second  $\text{Cu}^{\text{II}}$  ion is coordinated by the pyridyl N and two hydrazyl N atoms from different hydrazyl groups. The coordination environments of both  $\text{Cu}^{\text{II}}$  ions are completed by a chloride ion and a methanol molecule. The dihedral angle between the pyridyl groups is  $27.46(10)^\circ$ . The crystal packing is stabilized by  $\text{O}-\text{H}\cdots\text{O}$  (perchlorate),  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonding.

## Related literature

For the definition of the distortion parameter, see: Addison *et al.* (1984).



## Experimental

### Crystal data

$[\text{Cu}_2(\text{C}_{15}\text{H}_{15}\text{N}_6\text{O})\text{Cl}_2(\text{CH}_3\text{OH})_2]\text{ClO}_4$	$V = 5003.3(3) \text{ \AA}^3$
$M_r = 656.84$	$Z = 8$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 8.0319(3) \text{ \AA}$	$\mu = 2.07 \text{ mm}^{-1}$
$b = 16.6784(6) \text{ \AA}$	$T = 298 \text{ K}$
$c = 37.3492(13) \text{ \AA}$	$0.18 \times 0.16 \times 0.12 \text{ mm}$

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer	30236 measured reflections
Absorption correction: multi-scan ( <i>SHELXTL</i> ; Sheldrick, 2008)	5692 independent reflections
$T_{\text{min}} = 0.675$ , $T_{\text{max}} = 0.783$	4016 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.064$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	318 parameters
$wR(F^2) = 0.142$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.90 \text{ e \AA}^{-3}$
5692 reflections	$\Delta\rho_{\text{min}} = -0.67 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3B}\cdots\text{Cl1}^{\text{ii}}$	0.86	2.91	3.766 (4)	176
$\text{O1W}-\text{H1W}\cdots\text{Cl1}^{\text{ii}}$	1.01	2.31	3.205 (4)	147
$\text{O2W}-\text{H2W}\cdots\text{O7}^{\text{iii}}$	1.00	1.90	2.855 (6)	159

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2081).

## References

- Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.  
 Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

*Acta Cryst.* (2009). E65, m1347 [ doi:10.1107/S1600536809040471 ]

**{ $\mu$ -1,5-Bis[(*E*)-1-(2-pyridyl)ethylidene]carbonohydrazidato(1-)}bis[chloridomethanolcopper(II)] perchlorate**

**W. Huang**

**Comment**

Recent research has witnessed considerable interest in the development of new multidentate ligands. Polyamine tripod ligands containing appropriate binding sites and shape may be designed to form special topological structures. The molecular topology of the host molecule can be synthetically modulated to bind many different chemical species from transition metals to lanthanide ions. To this purpose, the title compound was synthesized and structurally characterized. It features a dinuclear copper(II) complex assembled from one mono-deprotonated, bis-tridentate ligand and two distinct copper(II) ions. The coordination of Cu1 is achieved by pyridyl-N, hydrazine-N (deprotonated hydrazine group) and carbonyl-O, Cu2 is coordinated by the second pyridyl-N, hydrazine-N and the second hydrazine-N of the first hydrazine group (Fig. 1). The coordination environments of both Cu<sup>II</sup> ions are completed by one chloride ion and one methanol molecule. Both of the copper atoms adopt similar distorted 4 + 1 coordinated square-pyramid geometries with a distortion parameter 0.197 for Cu1 and 0.101 for Cu2 (Addison *et al.*, 1984). The crystal packing is stabilised by O-H...O(perchlorate), O-H...Cl and N-H...Cl hydrogen bonding (Fig. 2) The dihedral angle between the pyridyl groups is 27.46 (10)°.

**Experimental**

A methanolic solution (15 ml) containing the ligand (0.1 mmol, 0.03 g) was added dropwise to a methanolic solution (10 ml) containing CuCl<sub>2</sub>·2H<sub>2</sub>O (0.1 mmol, 0.034 g). After stirring for 2 h, the solution was filtered. Dark-green block-shaped crystals suitable for single-crystal X-ray diffraction were obtained by evaporating the resulting filtration in air for several days (yield: 65.6% based on the ligand). Anal calc (%). for C<sub>17</sub>H<sub>23</sub>Cl<sub>3</sub>Cu<sub>2</sub>N<sub>6</sub>O<sub>7</sub>: H 3.53 C 31.09 N 12.79 Found: H 3.42, C 31.21, N 12.86.

**Refinement**

C-bound H atoms were placed geometrically and allowed to ride during refinement with C—H = 0.93–0.96 Å with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . O-bound H atoms were located in a difference Fourier map and refined as riding with the parent atom with an isotropic thermal parameter 1.5 times that of the parent atom.

**Figures**

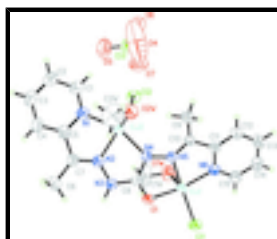


Fig. 1. The dinuclear cation and the perchlorate anion in the structure of the title compound. Thermal ellipsoids are drawn at the 50% level.

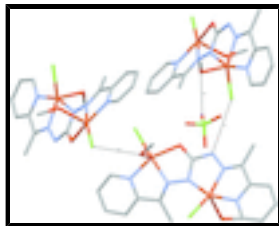


Fig. 2. The hydrogen bonding pattern in the title compound.

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### Crystal data

[Cu<sub>2</sub>(C<sub>15</sub>H<sub>15</sub>N<sub>6</sub>O)Cl<sub>2</sub>(CH<sub>4</sub>O)<sub>2</sub>]ClO<sub>4</sub>

$M_r = 656.84$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.0319 (3) \text{ \AA}$

$b = 16.6784 (6) \text{ \AA}$

$c = 37.3492 (13) \text{ \AA}$

$V = 5003.3 (3) \text{ \AA}^3$

$Z = 8$

$F_{000} = 2656$

$D_x = 1.744 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 15443 reflections

$\theta = 2.3\text{--}27.0^\circ$

$\mu = 2.07 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, dark-green

$0.18 \times 0.16 \times 0.12 \text{ mm}$

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298 \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SHELXTL; Sheldrick, 2008)

$T_{\min} = 0.675$ ,  $T_{\max} = 0.783$

30236 measured reflections

5692 independent reflections

4016 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.064$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 2.2^\circ$

$h = -10 \rightarrow 10$

$k = -21 \rightarrow 21$

$l = -48 \rightarrow 39$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.142$

$S = 1.04$

5692 reflections

318 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 3.3159P]$

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

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

$\Delta\rho_{\max} = 0.90 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.67 \text{ e \AA}^{-3}$

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

*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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.62011 (6)	0.28060 (3)	0.033586 (13)	0.03826 (15)
Cu2	0.81104 (6)	0.39647 (3)	0.143708 (12)	0.03630 (15)
C1	0.8701 (6)	0.4718 (3)	0.21601 (12)	0.0538 (11)
H1A	0.8464	0.5205	0.2050	0.065*
C1W	0.3072 (9)	0.2671 (5)	0.08697 (17)	0.112 (3)
H1WA	0.1939	0.2822	0.0916	0.167*
H1WB	0.3761	0.2840	0.1066	0.167*
H1WC	0.3143	0.2100	0.0844	0.167*
C2	0.9166 (7)	0.4715 (3)	0.25190 (13)	0.0610 (13)
H2A	0.9248	0.5191	0.2647	0.073*
C2W	1.2080 (7)	0.4315 (5)	0.1542 (2)	0.098 (2)
H2WA	1.3027	0.4607	0.1455	0.147*
H2WB	1.2250	0.3752	0.1504	0.147*
H2WC	1.1941	0.4417	0.1794	0.147*
C3	0.9502 (6)	0.3989 (3)	0.26802 (12)	0.0569 (12)
H3A	0.9802	0.3970	0.2921	0.068*
C4	0.9391 (5)	0.3293 (3)	0.24833 (11)	0.0486 (10)
H4A	0.9623	0.2799	0.2588	0.058*
C5	0.8929 (5)	0.3338 (3)	0.21264 (11)	0.0411 (9)
C6	0.8894 (7)	0.1789 (3)	0.20249 (13)	0.0591 (12)
H6A	0.8749	0.1424	0.1829	0.089*
H6B	0.8048	0.1694	0.2201	0.089*
H6C	0.9971	0.1708	0.2130	0.089*
C7	0.8762 (5)	0.2626 (3)	0.18923 (11)	0.0398 (9)
C8	0.7643 (5)	0.2622 (2)	0.09818 (10)	0.0368 (8)
C9	0.8716 (5)	0.4960 (3)	0.06034 (12)	0.0481 (10)
H9A	0.9033	0.4835	0.0845	0.072*
H9B	0.8118	0.5459	0.0600	0.072*
H9C	0.9695	0.5006	0.0457	0.072*
C10	0.7642 (4)	0.4315 (2)	0.04617 (10)	0.0346 (8)
C11	0.6971 (5)	0.4355 (2)	0.00899 (10)	0.0364 (8)

## supplementary materials

C12	0.7161 (5)	0.5001 (3)	-0.01319 (11)	0.0447 (10)
H12A	0.7704	0.5459	-0.0051	0.054*
C13	0.6538 (6)	0.4967 (3)	-0.04776 (13)	0.0543 (12)
H13A	0.6684	0.5398	-0.0633	0.065*
C14	0.5709 (6)	0.4299 (3)	-0.05879 (12)	0.0579 (12)
H14A	0.5266	0.4270	-0.0818	0.069*
C15	0.5539 (6)	0.3668 (3)	-0.03538 (11)	0.0491 (10)
H15A	0.4969	0.3213	-0.0429	0.059*
N1	0.8586 (4)	0.4049 (2)	0.19707 (9)	0.0411 (8)
N2	0.8459 (4)	0.28245 (19)	0.15635 (9)	0.0387 (7)
N3	0.8162 (5)	0.2289 (2)	0.12969 (9)	0.0424 (8)
H3B	0.8291	0.1781	0.1324	0.051*
N4	0.7825 (4)	0.34270 (19)	0.09563 (8)	0.0359 (7)
N5	0.7277 (4)	0.36484 (18)	0.06188 (8)	0.0340 (7)
N6	0.6157 (4)	0.3682 (2)	-0.00234 (9)	0.0392 (7)
O1	0.7099 (4)	0.21631 (15)	0.07431 (7)	0.0447 (7)
O1W	0.3611 (4)	0.3035 (2)	0.05585 (9)	0.0620 (9)
O2W	1.0641 (4)	0.45651 (19)	0.13568 (8)	0.0540 (8)
O4	0.2605 (8)	0.6862 (8)	0.1635 (3)	0.276 (6)
O5	0.1217 (13)	0.6334 (4)	0.20860 (15)	0.189 (4)
O6	0.0314 (10)	0.7448 (4)	0.17370 (16)	0.159 (3)
O7	0.0200 (11)	0.6230 (3)	0.15081 (16)	0.167 (3)
Cl1	0.54972 (14)	0.18014 (6)	-0.00266 (3)	0.0493 (3)
Cl2	0.64899 (14)	0.50485 (7)	0.13951 (3)	0.0529 (3)
Cl3	0.1126 (2)	0.66852 (9)	0.17526 (4)	0.0740 (4)
H1W	0.2879	0.2904	0.0347	0.089*
H2W	1.0197	0.5118	0.1398	0.089*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0495 (3)	0.0282 (3)	0.0371 (3)	-0.0014 (2)	-0.0063 (2)	-0.00165 (19)
Cu2	0.0432 (3)	0.0324 (3)	0.0332 (3)	0.0015 (2)	-0.00304 (19)	-0.00154 (19)
C1	0.063 (3)	0.047 (3)	0.051 (3)	-0.004 (2)	-0.004 (2)	-0.006 (2)
C1W	0.101 (5)	0.180 (8)	0.055 (4)	-0.031 (5)	0.007 (4)	0.014 (4)
C2	0.075 (3)	0.060 (3)	0.048 (3)	-0.006 (3)	-0.007 (2)	-0.013 (2)
C2W	0.051 (3)	0.128 (6)	0.115 (5)	0.007 (4)	-0.011 (3)	-0.010 (5)
C3	0.062 (3)	0.072 (4)	0.037 (2)	-0.005 (3)	-0.005 (2)	-0.004 (2)
C4	0.054 (2)	0.057 (3)	0.034 (2)	-0.004 (2)	-0.0024 (19)	0.0016 (19)
C5	0.038 (2)	0.048 (3)	0.037 (2)	-0.0022 (17)	0.0008 (16)	0.0019 (19)
C6	0.082 (3)	0.045 (3)	0.050 (3)	0.006 (2)	-0.002 (2)	0.007 (2)
C7	0.042 (2)	0.040 (2)	0.038 (2)	0.0016 (17)	0.0020 (17)	0.0037 (17)
C8	0.047 (2)	0.032 (2)	0.0311 (19)	-0.0011 (16)	0.0009 (16)	-0.0001 (16)
C9	0.055 (2)	0.040 (2)	0.050 (3)	-0.0123 (19)	-0.0035 (19)	0.0011 (19)
C10	0.0360 (19)	0.030 (2)	0.038 (2)	0.0001 (15)	0.0023 (16)	-0.0010 (16)
C11	0.0362 (19)	0.033 (2)	0.040 (2)	0.0052 (16)	0.0035 (16)	-0.0015 (16)
C12	0.051 (2)	0.037 (2)	0.046 (2)	0.0006 (18)	0.0006 (19)	0.0029 (18)
C13	0.067 (3)	0.049 (3)	0.047 (3)	0.013 (2)	0.002 (2)	0.015 (2)

C14	0.076 (3)	0.057 (3)	0.041 (2)	0.011 (3)	-0.013 (2)	0.002 (2)
C15	0.060 (3)	0.042 (2)	0.045 (2)	0.003 (2)	-0.015 (2)	0.0004 (19)
N1	0.0473 (19)	0.037 (2)	0.0389 (18)	-0.0001 (14)	-0.0046 (15)	-0.0018 (15)
N2	0.0471 (19)	0.0336 (18)	0.0355 (17)	-0.0011 (14)	-0.0040 (14)	-0.0013 (14)
N3	0.065 (2)	0.0291 (18)	0.0333 (17)	0.0030 (15)	-0.0065 (15)	0.0006 (14)
N4	0.0467 (18)	0.0319 (18)	0.0289 (16)	-0.0031 (14)	-0.0004 (13)	0.0008 (13)
N5	0.0393 (17)	0.0304 (17)	0.0322 (16)	0.0006 (13)	-0.0007 (13)	-0.0013 (13)
N6	0.0456 (18)	0.0320 (18)	0.0399 (18)	0.0011 (14)	-0.0058 (14)	-0.0006 (14)
O1	0.0696 (19)	0.0259 (14)	0.0386 (15)	-0.0030 (13)	-0.0103 (13)	-0.0012 (12)
O1W	0.060 (2)	0.069 (2)	0.057 (2)	0.0002 (16)	0.0050 (16)	0.0026 (17)
O2W	0.0486 (17)	0.055 (2)	0.0578 (19)	-0.0072 (15)	-0.0076 (14)	-0.0021 (15)
O4	0.077 (4)	0.488 (17)	0.263 (9)	-0.028 (7)	-0.029 (5)	0.232 (11)
O5	0.361 (11)	0.138 (5)	0.068 (3)	-0.100 (6)	-0.028 (5)	0.020 (3)
O6	0.242 (8)	0.129 (5)	0.108 (4)	0.047 (6)	-0.015 (5)	-0.033 (4)
O7	0.295 (9)	0.073 (3)	0.131 (5)	-0.026 (4)	-0.096 (5)	-0.015 (3)
Cl1	0.0617 (7)	0.0353 (6)	0.0509 (6)	-0.0058 (5)	-0.0110 (5)	-0.0075 (4)
Cl2	0.0561 (6)	0.0500 (7)	0.0526 (6)	0.0180 (5)	-0.0067 (5)	-0.0051 (5)
Cl3	0.0885 (10)	0.0661 (9)	0.0673 (9)	-0.0155 (7)	0.0015 (7)	-0.0110 (7)

*Geometric parameters (Å, °)*

Cu1—N5	1.959 (3)	C6—H6B	0.9600
Cu1—N6	1.985 (3)	C6—H6C	0.9600
Cu1—O1	1.996 (3)	C7—N2	1.294 (5)
Cu1—Cl1	2.2270 (11)	C8—O1	1.253 (4)
Cu1—O1W	2.273 (3)	C8—N4	1.354 (5)
Cu2—N2	1.979 (3)	C8—N3	1.367 (5)
Cu2—N4	2.020 (3)	C9—C10	1.477 (5)
Cu2—N1	2.034 (3)	C9—H9A	0.9600
Cu2—Cl2	2.2330 (11)	C9—H9B	0.9600
Cu2—O2W	2.285 (3)	C9—H9C	0.9600
C1—N1	1.324 (6)	C10—N5	1.292 (5)
C1—C2	1.392 (6)	C10—C11	1.491 (5)
C1—H1A	0.9300	C11—N6	1.366 (5)
C1W—O1W	1.380 (7)	C11—C12	1.367 (6)
C1W—H1WA	0.9600	C12—C13	1.386 (6)
C1W—H1WB	0.9600	C12—H12A	0.9300
C1W—H1WC	0.9600	C13—C14	1.362 (7)
C2—C3	1.378 (7)	C13—H13A	0.9300
C2—H2A	0.9300	C14—C15	1.375 (6)
C2W—O2W	1.411 (6)	C14—H14A	0.9300
C2W—H2WA	0.9600	C15—N6	1.330 (5)
C2W—H2WB	0.9600	C15—H15A	0.9300
C2W—H2WC	0.9600	N2—N3	1.358 (5)
C3—C4	1.378 (6)	N3—H3B	0.8600
C3—H3A	0.9300	N4—N5	1.386 (4)
C4—C5	1.386 (6)	O1W—H1W	1.0086
C4—H4A	0.9300	O2W—H2W	1.0003
C5—N1	1.349 (5)	O4—Cl3	1.301 (7)

## supplementary materials

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C5—C7	1.481 (6)	O5—C13	1.378 (6)
C6—C7	1.486 (6)	O6—C13	1.430 (7)
C6—H6A	0.9600	O7—C13	1.401 (5)
N5—Cu1—N6	81.04 (13)	O1—C8—N3	118.1 (4)
N5—Cu1—O1	79.33 (12)	N4—C8—N3	115.5 (3)
N6—Cu1—O1	156.56 (13)	C10—C9—H9A	109.5
N5—Cu1—C11	168.39 (10)	C10—C9—H9B	109.5
N6—Cu1—C11	97.97 (10)	H9A—C9—H9B	109.5
O1—Cu1—C11	98.68 (8)	C10—C9—H9C	109.5
N5—Cu1—O1W	94.93 (13)	H9A—C9—H9C	109.5
N6—Cu1—O1W	96.16 (13)	H9B—C9—H9C	109.5
O1—Cu1—O1W	98.17 (13)	N5—C10—C9	126.7 (4)
C11—Cu1—O1W	96.68 (10)	N5—C10—C11	112.3 (3)
N2—Cu2—N4	78.56 (13)	C9—C10—C11	120.8 (3)
N2—Cu2—N1	78.81 (14)	N6—C11—C12	120.8 (4)
N4—Cu2—N1	157.34 (13)	N6—C11—C10	115.2 (3)
N2—Cu2—C12	151.28 (11)	C12—C11—C10	124.0 (4)
N4—Cu2—C12	103.35 (10)	C11—C12—C13	119.5 (4)
N1—Cu2—C12	97.03 (10)	C11—C12—H12A	120.2
N2—Cu2—O2W	109.06 (13)	C13—C12—H12A	120.2
N4—Cu2—O2W	100.30 (12)	C14—C13—C12	119.4 (4)
N1—Cu2—O2W	86.07 (13)	C14—C13—H13A	120.3
C12—Cu2—O2W	98.88 (9)	C12—C13—H13A	120.3
N1—C1—C2	122.0 (5)	C13—C14—C15	118.9 (4)
N1—C1—H1A	119.0	C13—C14—H14A	120.6
C2—C1—H1A	119.0	C15—C14—H14A	120.6
O1W—C1W—H1WA	109.5	N6—C15—C14	122.6 (4)
O1W—C1W—H1WB	109.5	N6—C15—H15A	118.7
H1WA—C1W—H1WB	109.5	C14—C15—H15A	118.7
O1W—C1W—H1WC	109.5	C1—N1—C5	119.7 (4)
H1WA—C1W—H1WC	109.5	C1—N1—Cu2	126.5 (3)
H1WB—C1W—H1WC	109.5	C5—N1—Cu2	113.6 (3)
C3—C2—C1	118.5 (5)	C7—N2—N3	124.1 (3)
C3—C2—H2A	120.8	C7—N2—Cu2	119.9 (3)
C1—C2—H2A	120.8	N3—N2—Cu2	115.6 (2)
O2W—C2W—H2WA	109.5	N2—N3—C8	114.7 (3)
O2W—C2W—H2WB	109.5	N2—N3—H3B	122.6
H2WA—C2W—H2WB	109.5	C8—N3—H3B	122.6
O2W—C2W—H2WC	109.5	C8—N4—N5	107.1 (3)
H2WA—C2W—H2WC	109.5	C8—N4—Cu2	113.0 (2)
H2WB—C2W—H2WC	109.5	N5—N4—Cu2	136.6 (2)
C4—C3—C2	119.6 (4)	C10—N5—N4	124.8 (3)
C4—C3—H3A	120.2	C10—N5—Cu1	118.2 (3)
C2—C3—H3A	120.2	N4—N5—Cu1	116.1 (2)
C3—C4—C5	119.0 (4)	C15—N6—C11	118.7 (4)
C3—C4—H4A	120.5	C15—N6—Cu1	128.4 (3)
C5—C4—H4A	120.5	C11—N6—Cu1	112.8 (2)
N1—C5—C4	121.2 (4)	C8—O1—Cu1	109.9 (2)
N1—C5—C7	115.5 (3)	C1W—O1W—Cu1	121.4 (4)



C4—C5—C7	123.3 (4)	C1W—O1W—H1W	112.5
C7—C6—H6A	109.5	Cu1—O1W—H1W	102.2
C7—C6—H6B	109.5	C2W—O2W—Cu2	122.3 (4)
H6A—C6—H6B	109.5	C2W—O2W—H2W	119.3
C7—C6—H6C	109.5	Cu2—O2W—H2W	93.8
H6A—C6—H6C	109.5	O4—Cl3—O5	110.7 (5)
H6B—C6—H6C	109.5	O4—Cl3—O7	112.7 (7)
N2—C7—C5	111.9 (4)	O5—Cl3—O7	112.7 (4)
N2—C7—C6	124.7 (4)	O4—Cl3—O6	101.6 (6)
C5—C7—C6	123.4 (4)	O5—Cl3—O6	116.0 (5)
O1—C8—N4	126.4 (3)	O7—Cl3—O6	102.3 (4)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3B $\cdots$ Cl2 <sup>i</sup>	0.86	2.91	3.766 (4)	176
O1W—H1W $\cdots$ Cl1 <sup>ii</sup>	1.01	2.31	3.205 (4)	147
O2W—H2W $\cdots$ O7 <sup>iii</sup>	1.00	1.90	2.855 (6)	159

Symmetry codes: (i)  $-x+3/2, y-1/2, z$ ; (ii)  $x-1/2, -y+1/2, -z$ ; (iii)  $x+1, y, z$ .

Fig. 1

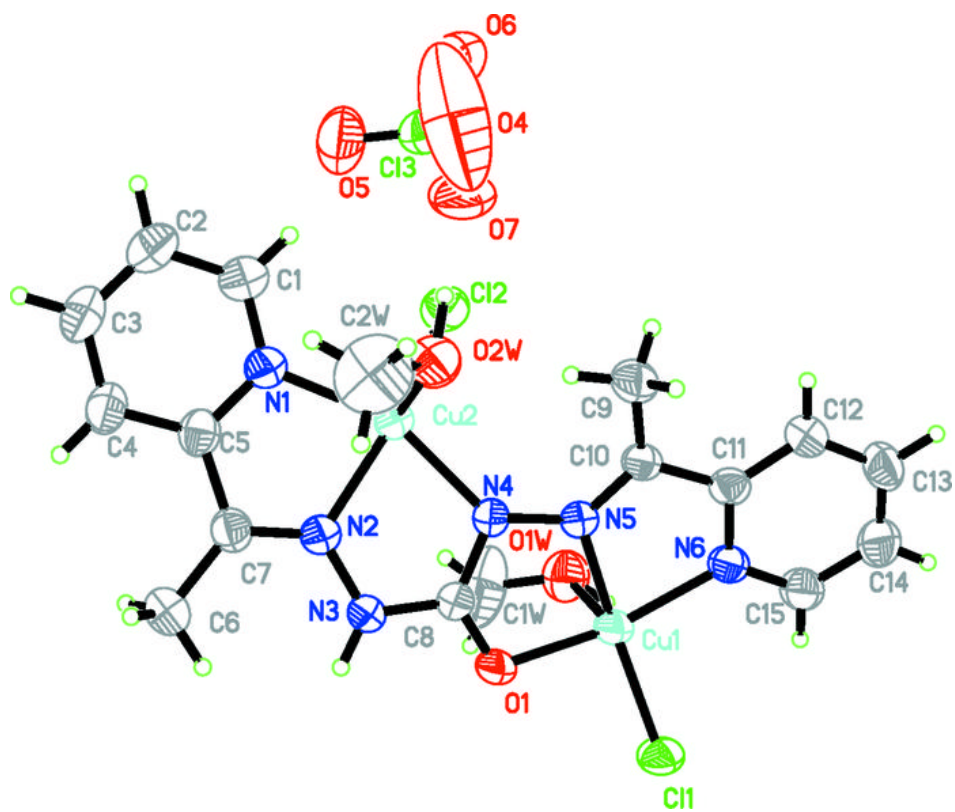


Fig. 2

