

## ( $\mu$ -3,4:9,10:17,18:23,24-Tetrabenzo-1,12,15,26-tetraaza-5,8,19,22-tetraoxacyclooctacosane- $\kappa^4N^1, N^{26}:-N^{12}, N^{15}$ )bis[aquadichloridocopper(II)]

Zhi-Fang Jia, Jian-Fang Ma,\* Lai-Ping Zhang and Ting-Ting Han

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: majf247nenu@yahoo.com.cn

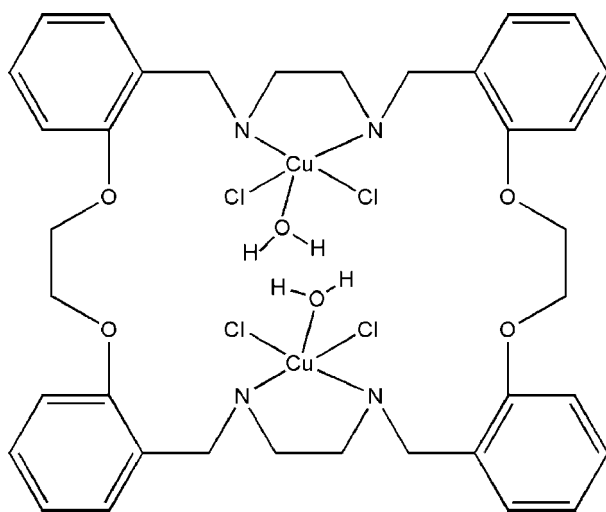
Received 25 September 2007; accepted 28 September 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.142; data-to-parameter ratio = 14.1.

In the title compound,  $[\text{Cu}_2\text{Cl}_4(\text{C}_{36}\text{H}_{44}\text{N}_4\text{O}_4)(\text{H}_2\text{O})_2]$ , the dinuclear complex molecule lies on an inversion centre. Each  $\text{Cu}^{\text{II}}$  atom shows a tetragonal-pyramidal coordination geometry formed by two Cl atoms, two N atoms from the macrocyclic ligand and one water molecule. The coordinated water molecules are hydrogen-bonded to the Cl atoms in adjacent molecules, generating a one-dimensional structure.

### Related literature

For related literature, see: Adam *et al.* (1981); Barczynski *et al.* (2007); Davis *et al.* (1995); Higa *et al.* (2007); Jiang *et al.* (2007); Michalska *et al.* (2007); Zhou *et al.* (2007).



### Experimental

#### Crystal data

$[\text{Cu}_2\text{Cl}_4(\text{C}_{36}\text{H}_{44}\text{N}_4\text{O}_4)(\text{H}_2\text{O})_2]$   
 $M_r = 901.66$

Monoclinic,  $P2_1/n$

$a = 13.193$  (1) Å

$b = 8.4530$  (8) Å

$c = 17.913$  (2) Å

$\beta = 98.211$  (2)°

$V = 1977.2$  (3) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 1.40$  mm<sup>-1</sup>

$T = 293$  (2) K

$0.45 \times 0.36 \times 0.24$  mm

#### Data collection

Bruker SMART APEX CCD  
 area-detector diffractometer

Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)

$T_{\text{min}} = 0.55$ ,  $T_{\text{max}} = 0.72$

9616 measured reflections

3493 independent reflections

2151 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

#### Refinement

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

$wR(F^2) = 0.142$

$S = 1.01$

3493 reflections

247 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.47$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.46$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1—N1	2.035 (4)	Cu1—O1W	2.303 (4)
Cu1—N2	2.044 (4)	Cu1—Cl2	2.3078 (15)
Cu1—Cl1	2.2964 (15)		
N1—Cu1—N2	84.17 (17)	Cl1—Cu1—O1W	96.31 (11)
N1—Cu1—Cl1	164.46 (13)	N1—Cu1—Cl2	88.39 (12)
N2—Cu1—Cl1	90.30 (13)	N2—Cu1—Cl2	169.54 (13)
N1—Cu1—O1W	98.39 (16)	Cl1—Cu1—Cl2	94.99 (5)
N2—Cu1—O1W	92.11 (16)	O1W—Cu1—Cl2	96.26 (11)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1B $\cdots$ Cl1 <sup>i</sup>	1.00 (4)	2.22 (5)	3.152 (4)	155 (5)
O1W—H1A $\cdots$ Cl2 <sup>i</sup>	0.81 (4)	2.47 (5)	3.215 (4)	154 (6)

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Siemens, 1990); software used to prepare material for publication: SHELXL97.

The authors thank the National Natural Science Foundation of China (grant No. 20471014), the Programme for New Century Excellent Talents in Chinese University (grant No. NCET-05-0320), the Fok Ying Tung Education Foundation and the Analysis and Testing Foundation of Northeast Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2086).

## References

- Adam, K. R., Anderegg, G., Henrick, K., Leong, A. J., Lindoy, L. F., Lip, H. C., Mcpartlin, M., Smith, R. J. & Tasker, P. A. (1981). *Inorg. Chem.* **20**, 4048–4053.
- Barczynski, P., Komasa, A., Katrusiak, A., Dega-Szafran, Z. & Szafran, M. (2007). *J. Mol. Struct.* **832**, 63–72.
- Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINTE*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
- Davis, C. A., Duckworth, P. A., Lingdoy, L. F. & Moody, W. E. (1995). *Aust. J. Chem.* **48**, 1819–1825.
- Higa, T., Moriya, M., Shimazaki, Y., Yajima, T., Tani, F., Karasawa, S., Nakano, M., Naruta, Y. & Yamauchi, O. (2007). *Inorg. Chim. Acta*, **360**, 3304–3313.
- Jiang, H., Ma, J.-F. & Zhang, W.-L. (2007). *Acta Cryst.* **E63**, m1681.
- Michalska, D., Hernik, K., Wysokinski, R., Morzyk-Ociepa, B. & Pietraszko, A. (2007). *Polyhedron*, **26**, 4303–4313.
- Sheldrick, G. M. (1996). *SADABS*. Version 2.03. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Siemens (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Zhou, X. L., Meng, X. R., Cheng, W., Hou, H. W., Tang, M. S. & Fan, Y. T. (2007). *Inorg. Chim. Acta*, **360**, 3467–3474.

**supplementary materials**

*Acta Cryst.* (2007). E63, m2652-m2653 [ doi:10.1107/S1600536807047678 ]

**( $\mu$ -3,4:9,10:17,18:23,24-Tetrabenzo-1,12,15,26-tetraaza-5,8,19,22-tetraoxacyclooctacosane- $\kappa^4 N^1, N^{26}; N^{12}, N^{15}$ )bis[aquadichloridocopper(II)]**

**Z.-F. Jia, J.-F. Ma, L.-P. Zhang and T.-T. Han**

### Comment

The use of macrocyclic ligands for the formation of selective metal complex has received considerable attention over many years (Davis *et al.*, 1995). The method for the synthesis of the title complex has been reported (Adam *et al.*, 1981). However, to the best of our knowledge, the crystal structure has not been reported yet.

The molecule of the title compound is composed of two  $\text{Cu}^{\text{II}}$  atoms, four  $\text{Cl}^-$  atoms, a 3,4:9,10:17,18:23,24-tetrabenzo-1,12,15,26-tetraaza-5,8,19,22-tetraoxacyclooctacosane (*L*) ligand and two water molecules (Fig.1). It is a centrosymmetric molecule. Each  $\text{Cu}^{\text{II}}$  atom shows a tetragonal-pyramidal coordination geometry, formed by two  $\text{Cl}^-$  atoms, two N atoms from *L* and one water molecule. The bond distances and angles show normal values (Table 1) (Higa *et al.*, 2007; Jiang *et al.*, 2007; Michalska *et al.*, 2007; Zhou *et al.*, 2007). There are hydrogen-bonding interactions in the crystal structure. As shown in Fig. 2 and in Table 2, there are two O—H $\cdots$ Cl hydrogen bonds between the water molecule and  $\text{Cl}^-$  atoms, leading to a one-dimensional supramolecular structure (Barczynski *et al.*, 2007).

### Experimental

*L* (0.100 g, 0.17 mmol) dissolved in hot ethanol (15 ml) was added to a solution of  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  (0.030 g, 0.17 mmol) in hot water (10 ml). After stirring for 30 min, the mixture was filtered. Blue single crystals of the title compound were obtained after several days at room temperature.

### Refinement

All H atoms bound to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å (CH) and 0.97 Å ( $\text{CH}_2$ ) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms bound to N atoms and belonging to water molecule were located in a difference Fourier map and refined with  $U_{\text{iso}}(\text{H}) = 1.4U_{\text{eq}}(\text{N})$  and  $U_{\text{iso}}(\text{H}) = 1.3U_{\text{eq}}(\text{O})$ , respectively.

### Figures

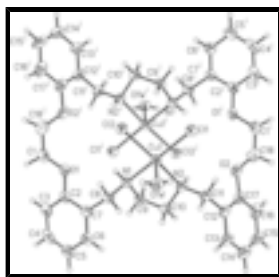


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 - x, 1 - y, 1 - z.]

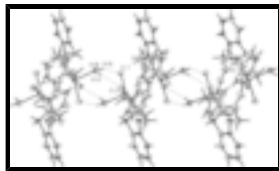


Fig. 2. One-dimensional structure in the title compound. Hydrogen bonds are shown as dashed lines. Displacement ellipsoids are drawn at the 30% probability level.

**( $\mu$ -3,4:9,10:17,18:23,24-Tetrabenzo-1,12,15,26-tetraaza-5,8,19,22-tetraoxacyclooctacosane- $\kappa^4 N^1, N^{26}; N^{12}, N^{15}$ )bis[aquadichloridocopper(II)]**

### Crystal data

[Cu<sub>2</sub>Cl<sub>4</sub>(C<sub>36</sub>H<sub>44</sub>N<sub>4</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 901.66$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 13.193$  (1) Å

$b = 8.4530$  (8) Å

$c = 17.913$  (2) Å

$\beta = 98.211$  (2)°

$V = 1977.2$  (3) Å<sup>3</sup>

$Z = 2$

$F_{000} = 932$

$D_x = 1.515$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3493 reflections

$\theta = 1.8$ – $25.1$ °

$\mu = 1.40$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, blue

$0.45 \times 0.36 \times 0.24$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.55$ ,  $T_{\max} = 0.72$

9616 measured reflections

3493 independent reflections

2151 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\text{max}} = 25.1$ °

$\theta_{\text{min}} = 1.8$ °

$h = -15 \rightarrow 14$

$k = -10 \rightarrow 9$

$l = -10 \rightarrow 21$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

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

$wR(F^2) = 0.142$

$S = 1.01$

3493 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2]$$

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

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

$\Delta\rho_{\text{max}} = 0.47$  e Å<sup>-3</sup>

247 parameters

$$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$$

2 restraints

Extinction correction: none

Primary atom site location: structure-invariant direct methods

### 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.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.44875 (4)	0.70615 (7)	0.52017 (3)	0.0447 (2)
C1	0.2640 (5)	0.4791 (7)	0.2253 (3)	0.0617 (15)
H7A	0.2055	0.5058	0.1883	0.074*
H7B	0.2647	0.3652	0.2320	0.074*
C2	0.1616 (4)	0.5391 (6)	0.3202 (3)	0.0517 (14)
C3	0.0785 (5)	0.4584 (7)	0.2829 (4)	0.0673 (17)
H4	0.0833	0.4084	0.2373	0.081*
C4	-0.0119 (5)	0.4520 (8)	0.3135 (5)	0.084 (2)
H3	-0.0670	0.3950	0.2887	0.101*
C5	-0.0218 (5)	0.5281 (9)	0.3794 (4)	0.085 (2)
H2	-0.0832	0.5243	0.3992	0.103*
C6	0.0609 (4)	0.6105 (8)	0.4161 (4)	0.0679 (17)
H1	0.0542	0.6631	0.4607	0.082*
C7	0.1536 (4)	0.6171 (6)	0.3884 (3)	0.0521 (14)
C8	0.2442 (4)	0.7015 (6)	0.4312 (3)	0.0506 (13)
H16A	0.2763	0.7660	0.3964	0.061*
H16B	0.2207	0.7715	0.4680	0.061*
C9	0.2833 (4)	0.4900 (6)	0.5276 (3)	0.0559 (15)
H17A	0.3217	0.3918	0.5332	0.067*
H17B	0.2117	0.4646	0.5118	0.067*
C10	0.2949 (4)	0.5753 (7)	0.6006 (3)	0.0566 (15)
H18A	0.2786	0.5053	0.6402	0.068*
H18B	0.2484	0.6647	0.5974	0.068*
C11	0.5860 (4)	0.2581 (6)	0.3172 (3)	0.0560 (15)
H15A	0.5168	0.2164	0.3097	0.067*
H15B	0.6327	0.1700	0.3288	0.067*
C12	0.6074 (5)	0.3359 (7)	0.2453 (3)	0.0585 (15)
C13	0.6979 (5)	0.3074 (8)	0.2161 (4)	0.0751 (19)
H14	0.7472	0.2411	0.2420	0.090*
C14	0.7156 (6)	0.3762 (10)	0.1493 (4)	0.088 (2)
H13	0.7751	0.3525	0.1293	0.106*
C15	0.6462 (7)	0.4785 (10)	0.1127 (4)	0.096 (3)
H12	0.6601	0.5272	0.0688	0.116*

## supplementary materials

---

C16	0.5547 (6)	0.5120 (8)	0.1396 (4)	0.083 (2)
H11	0.5073	0.5818	0.1142	0.099*
C17	0.5361 (5)	0.4361 (7)	0.2071 (3)	0.0638 (17)
C18	0.3590 (5)	0.5285 (7)	0.1969 (3)	0.0703 (18)
H8A	0.3551	0.5001	0.1441	0.084*
H8B	0.3665	0.6424	0.2010	0.084*
N1	0.3214 (3)	0.5906 (5)	0.4705 (2)	0.0453 (11)
N2	0.4025 (3)	0.6311 (5)	0.6184 (3)	0.0472 (11)
O1	0.2538 (3)	0.5538 (4)	0.2951 (2)	0.0561 (10)
O2	0.4457 (3)	0.4535 (5)	0.2392 (2)	0.0693 (11)
O1W	0.3772 (3)	0.9524 (4)	0.5303 (2)	0.0613 (11)
Cl1	0.60735 (10)	0.76791 (17)	0.58394 (8)	0.0568 (4)
Cl2	0.49428 (10)	0.74432 (16)	0.40179 (8)	0.0546 (4)
H1C	0.336 (4)	0.521 (6)	0.434 (3)	0.065*
H2C	0.437 (4)	0.555 (6)	0.631 (3)	0.065*
H1A	0.411 (4)	1.010 (7)	0.560 (3)	0.082*
H1B	0.361 (4)	1.029 (6)	0.488 (3)	0.082*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0428 (4)	0.0478 (4)	0.0444 (4)	-0.0036 (3)	0.0096 (3)	-0.0014 (3)
C1	0.066 (4)	0.062 (4)	0.053 (4)	0.007 (3)	-0.006 (3)	-0.004 (3)
C2	0.043 (3)	0.052 (3)	0.057 (4)	0.001 (3)	-0.002 (3)	0.007 (3)
C3	0.064 (4)	0.058 (4)	0.073 (4)	-0.007 (3)	-0.013 (4)	-0.001 (3)
C4	0.049 (4)	0.086 (5)	0.106 (6)	-0.013 (3)	-0.024 (4)	0.025 (5)
C5	0.052 (4)	0.113 (6)	0.090 (6)	-0.010 (4)	0.006 (4)	0.024 (5)
C6	0.055 (4)	0.085 (5)	0.062 (4)	0.008 (3)	0.006 (3)	0.009 (3)
C7	0.043 (3)	0.056 (3)	0.057 (4)	0.000 (3)	0.005 (3)	0.007 (3)
C8	0.049 (3)	0.052 (3)	0.051 (3)	0.004 (3)	0.008 (3)	-0.003 (3)
C9	0.049 (3)	0.059 (4)	0.058 (4)	-0.008 (3)	0.005 (3)	0.001 (3)
C10	0.052 (3)	0.066 (4)	0.053 (4)	-0.011 (3)	0.012 (3)	0.002 (3)
C11	0.057 (3)	0.058 (4)	0.056 (3)	-0.004 (3)	0.018 (3)	-0.005 (3)
C12	0.071 (4)	0.061 (4)	0.046 (3)	-0.016 (3)	0.019 (3)	-0.009 (3)
C13	0.069 (4)	0.094 (5)	0.069 (4)	-0.022 (4)	0.033 (4)	-0.023 (4)
C14	0.089 (6)	0.100 (6)	0.084 (6)	-0.027 (5)	0.045 (5)	-0.027 (5)
C15	0.116 (7)	0.111 (7)	0.076 (5)	-0.043 (5)	0.062 (5)	-0.016 (5)
C16	0.114 (6)	0.075 (5)	0.061 (4)	-0.023 (4)	0.018 (4)	0.006 (4)
C17	0.081 (5)	0.061 (4)	0.053 (4)	-0.018 (3)	0.021 (4)	-0.013 (3)
C18	0.096 (5)	0.057 (4)	0.060 (4)	0.001 (4)	0.016 (4)	0.001 (3)
N1	0.040 (2)	0.052 (3)	0.043 (3)	-0.002 (2)	0.005 (2)	0.002 (2)
N2	0.049 (3)	0.047 (3)	0.048 (3)	-0.006 (2)	0.015 (2)	-0.005 (2)
O1	0.056 (2)	0.062 (2)	0.049 (2)	-0.0024 (18)	0.002 (2)	-0.0123 (19)
O2	0.076 (3)	0.087 (3)	0.048 (2)	0.007 (2)	0.019 (2)	0.006 (2)
O1W	0.065 (3)	0.055 (3)	0.068 (3)	-0.003 (2)	0.022 (2)	-0.006 (2)
Cl1	0.0484 (8)	0.0649 (9)	0.0568 (8)	-0.0073 (6)	0.0069 (7)	-0.0017 (7)
Cl2	0.0542 (8)	0.0645 (9)	0.0464 (7)	-0.0070 (6)	0.0121 (7)	0.0024 (7)

*Geometric parameters (Å, °)*

Cu1—N1	2.035 (4)	C9—H17B	0.9700
Cu1—N2	2.044 (4)	C10—N2	1.486 (6)
Cu1—C11	2.2964 (15)	C10—H18A	0.9700
Cu1—O1W	2.303 (4)	C10—H18B	0.9700
Cu1—C12	2.3078 (15)	C11—N2 <sup>i</sup>	1.477 (7)
C1—O1	1.425 (6)	C11—C12	1.507 (7)
C1—C18	1.479 (7)	C11—H15A	0.9700
C1—H7A	0.9700	C11—H15B	0.9700
C1—H7B	0.9700	C12—C17	1.373 (8)
C2—O1	1.362 (6)	C12—C13	1.392 (7)
C2—C3	1.380 (7)	C13—C14	1.381 (9)
C2—C7	1.406 (7)	C13—H14	0.9300
C3—C4	1.382 (8)	C14—C15	1.357 (10)
C3—H4	0.9300	C14—H13	0.9300
C4—C5	1.368 (9)	C15—C16	1.391 (9)
C4—H3	0.9300	C15—H12	0.9300
C5—C6	1.379 (9)	C16—C17	1.421 (8)
C5—H2	0.9300	C16—H11	0.9300
C6—C7	1.385 (7)	C17—O2	1.403 (6)
C6—H1	0.9300	C18—O2	1.427 (7)
C7—C8	1.504 (7)	C18—H8A	0.9700
C8—N1	1.485 (6)	C18—H8B	0.9700
C8—H16A	0.9700	N1—H1C	0.93 (5)
C8—H16B	0.9700	N2—C11 <sup>i</sup>	1.477 (7)
C9—N1	1.474 (6)	N2—H2C	0.80 (5)
C9—C10	1.481 (7)	O1W—H1A	0.81 (4)
C9—H17A	0.9700	O1W—H1B	1.00 (4)
N1—Cu1—N2	84.17 (17)	N2—C10—H18B	110.0
N1—Cu1—C11	164.46 (13)	H18A—C10—H18B	108.3
N2—Cu1—C11	90.30 (13)	N2 <sup>i</sup> —C11—C12	112.3 (4)
N1—Cu1—O1W	98.39 (16)	N2 <sup>i</sup> —C11—H15A	109.1
N2—Cu1—O1W	92.11 (16)	C12—C11—H15A	109.1
C11—Cu1—O1W	96.31 (11)	N2 <sup>i</sup> —C11—H15B	109.1
N1—Cu1—C12	88.39 (12)	C12—C11—H15B	109.1
N2—Cu1—C12	169.54 (13)	H15A—C11—H15B	107.9
C11—Cu1—C12	94.99 (5)	C17—C12—C13	118.9 (6)
O1W—Cu1—C12	96.26 (11)	C17—C12—C11	119.7 (5)
O1—C1—C18	111.6 (5)	C13—C12—C11	121.4 (6)
O1—C1—H7A	109.3	C14—C13—C12	120.9 (7)
C18—C1—H7A	109.3	C14—C13—H14	119.6
O1—C1—H7B	109.3	C12—C13—H14	119.6
C18—C1—H7B	109.3	C15—C14—C13	120.1 (7)
H7A—C1—H7B	108.0	C15—C14—H13	120.0
O1—C2—C3	124.9 (6)	C13—C14—H13	120.0
O1—C2—C7	115.1 (5)	C14—C15—C16	121.4 (7)



## supplementary materials

---

C3—C2—C7	120.0 (5)	C14—C15—H12	119.3
C2—C3—C4	119.9 (6)	C16—C15—H12	119.3
C2—C3—H4	120.0	C15—C16—C17	117.8 (7)
C4—C3—H4	120.0	C15—C16—H11	121.1
C5—C4—C3	121.2 (7)	C17—C16—H11	121.1
C5—C4—H3	119.4	C12—C17—O2	115.0 (5)
C3—C4—H3	119.4	C12—C17—C16	120.9 (6)
C4—C5—C6	118.8 (6)	O2—C17—C16	124.2 (6)
C4—C5—H2	120.6	O2—C18—C1	110.3 (5)
C6—C5—H2	120.6	O2—C18—H8A	109.6
C5—C6—C7	122.0 (6)	C1—C18—H8A	109.6
C5—C6—H1	119.0	O2—C18—H8B	109.6
C7—C6—H1	119.0	C1—C18—H8B	109.6
C6—C7—C2	118.1 (5)	H8A—C18—H8B	108.1
C6—C7—C8	121.0 (5)	C9—N1—C8	114.5 (4)
C2—C7—C8	120.8 (5)	C9—N1—Cu1	108.4 (3)
N1—C8—C7	112.5 (4)	C8—N1—Cu1	111.8 (3)
N1—C8—H16A	109.1	C9—N1—H1C	105 (3)
C7—C8—H16A	109.1	C8—N1—H1C	105 (3)
N1—C8—H16B	109.1	Cu1—N1—H1C	112 (3)
C7—C8—H16B	109.1	C11 <sup>i</sup> —N2—C10	110.9 (4)
H16A—C8—H16B	107.8	C11 <sup>i</sup> —N2—Cu1	117.8 (3)
N1—C9—C10	109.2 (4)	C10—N2—Cu1	107.9 (3)
N1—C9—H17A	109.8	C11 <sup>i</sup> —N2—H2C	107 (4)
C10—C9—H17A	109.8	C10—N2—H2C	107 (4)
N1—C9—H17B	109.8	Cu1—N2—H2C	106 (4)
C10—C9—H17B	109.8	C2—O1—C1	116.7 (4)
H17A—C9—H17B	108.3	C17—O2—C18	119.5 (5)
C9—C10—N2	108.6 (4)	Cu1—O1W—H1A	113 (5)
C9—C10—H18A	110.0	Cu1—O1W—H1B	125 (3)
N2—C10—H18A	110.0	H1A—O1W—H1B	99 (5)
C9—C10—H18B	110.0		
O1—C2—C3—C4	-179.6 (5)	C10—C9—N1—C8	-86.8 (5)
C7—C2—C3—C4	-1.2 (8)	C10—C9—N1—Cu1	38.8 (5)
C2—C3—C4—C5	1.8 (10)	C7—C8—N1—C9	-61.3 (6)
C3—C4—C5—C6	-0.9 (11)	C7—C8—N1—Cu1	175.0 (3)
C4—C5—C6—C7	-0.6 (10)	N2—Cu1—N1—C9	-13.3 (3)
C5—C6—C7—C2	1.1 (9)	C11—Cu1—N1—C9	56.3 (6)
C5—C6—C7—C8	-177.2 (6)	O1W—Cu1—N1—C9	-104.6 (3)
O1—C2—C7—C6	178.3 (5)	C12—Cu1—N1—C9	159.3 (3)
C3—C2—C7—C6	-0.3 (8)	N2—Cu1—N1—C8	113.8 (3)
O1—C2—C7—C8	-3.3 (7)	C11—Cu1—N1—C8	-176.5 (3)
C3—C2—C7—C8	178.1 (5)	O1W—Cu1—N1—C8	22.5 (3)
C6—C7—C8—N1	103.8 (6)	C12—Cu1—N1—C8	-73.6 (3)
C2—C7—C8—N1	-74.6 (6)	C9—C10—N2—C11 <sup>i</sup>	169.4 (4)
N1—C9—C10—N2	-52.1 (6)	C9—C10—N2—Cu1	39.0 (5)
N2 <sup>i</sup> —C11—C12—C17	-75.4 (7)	N1—Cu1—N2—C11 <sup>i</sup>	-140.6 (4)

N2 <sup>i</sup> —C11—C12—C13	105.2 (6)	C11—Cu1—N2—C11 <sup>i</sup>	54.0 (4)
C17—C12—C13—C14	-1.0 (9)	O1W—Cu1—N2—C11 <sup>i</sup>	-42.3 (4)
C11—C12—C13—C14	178.4 (6)	C12—Cu1—N2—C11 <sup>i</sup>	174.5 (5)
C12—C13—C14—C15	2.8 (10)	N1—Cu1—N2—C10	-14.1 (3)
C13—C14—C15—C16	-2.4 (11)	C11—Cu1—N2—C10	-179.5 (3)
C14—C15—C16—C17	0.3 (10)	O1W—Cu1—N2—C10	84.2 (3)
C13—C12—C17—O2	177.9 (5)	C12—Cu1—N2—C10	-59.0 (9)
C11—C12—C17—O2	-1.5 (8)	C3—C2—O1—C1	-0.2 (7)
C13—C12—C17—C16	-1.1 (9)	C7—C2—O1—C1	-178.7 (5)
C11—C12—C17—C16	179.5 (5)	C18—C1—O1—C2	169.0 (5)
C15—C16—C17—C12	1.5 (9)	C12—C17—O2—C18	-167.5 (5)
C15—C16—C17—O2	-177.4 (6)	C16—C17—O2—C18	11.4 (8)
O1—C1—C18—O2	74.8 (6)	C1—C18—O2—C17	157.1 (5)

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

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

<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>
O1W—H1B $\cdots$ C11 <sup>ii</sup>	1.00 (4)	2.22 (5)	3.152 (4)	155 (5)
O1W—H1A $\cdots$ C12 <sup>ii</sup>	0.81 (4)	2.47 (5)	3.215 (4)	154 (6)

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

Fig. 1

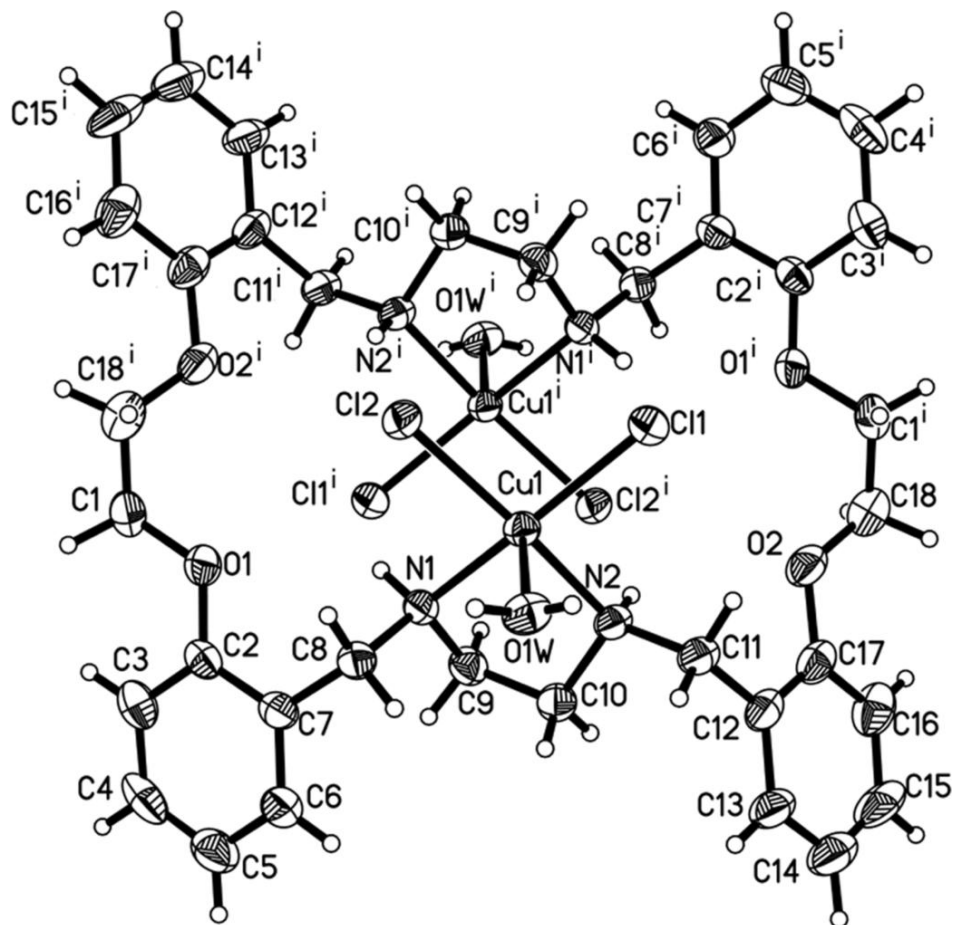


Fig. 2

