

# Bis(2-{1-[2-(2-hydroxyethylamino)ethyl-imino]propyl}phenolato)-1 $\kappa^4$ O,N,N',O';-2 $\kappa^4$ O,N,N',O'-methanol-2 $\kappa$ O- $\mu$ -perchlorato-1:2 $\kappa^2$ O:O'-perchlorato-1 $\kappa$ O-dicopper(II)

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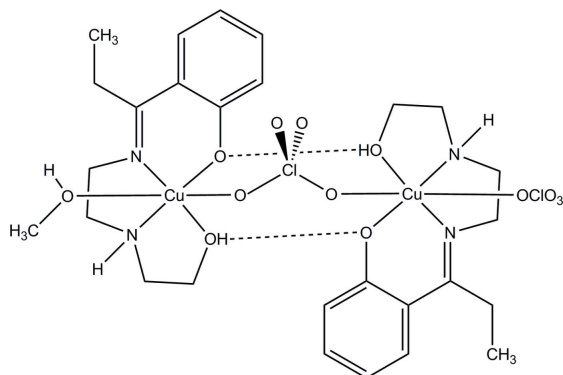
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å; some non-H atoms missing; disorder in main residue;  $R$  factor = 0.083;  $wR$  factor = 0.190; data-to-parameter ratio = 14.2.

The title compound,  $[\text{Cu}_2(\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_2)_2(\text{ClO}_4)_2(\text{CH}_4\text{O})]$ , consists of two six-coordinate Jahn–Teller-distorted copper(II) complex units with the tetradentate ligand 2-[1-[2-(2-hydroxyethylamino)ethylimino]propyl]phenolate observed in a planar coordination mode. Each copper center has octahedral coordination geometry. The complex units are axially connected by a bridging perchlorate anion. For one copper center, the other axial position is occupied by a terminal methanol molecule, while for the other copper center, the axial position is occupied by a weakly coordinated second perchlorate anion. As well as intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, the two Cu complex units are also linked by intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions. The four O atoms of one perchlorate are disordered over four positions; the site occupancy factors are 0.43, 0.25, 0.19 and 0.13.

## Related literature

For related literature, see: Butcher & Towns (2005); Cros *et al.* (1987); Plass *et al.* (2001); Swamy *et al.* (2001).



## Experimental

### Crystal data

$[\text{Cu}_2(\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_2)_2(\text{ClO}_4)_2(\text{CH}_4\text{O})]$   $V = 3401$  (2) Å<sup>3</sup>  
 $M_r = 828.63$   $Z = 4$   
Monoclinic,  $P2_1/n$  Mo  $K\alpha$  radiation  
 $a = 13.405$  (4) Å  $\mu = 1.48$  mm<sup>-1</sup>  
 $b = 13.154$  (5) Å  $T = 293$  (2) K  
 $c = 20.019$  (6) Å  $0.45 \times 0.40 \times 0.27$  mm  
 $\beta = 105.52$  (3)°

### Data collection

Bruker *P4* diffractometer 7797 independent reflections  
Absorption correction:  $\psi$  scans 4119 reflections with  $I > 2\sigma(I)$   
(North *et al.*, 1968)  $R_{\text{int}} = 0.048$   
 $T_{\text{min}} = 0.634$ ,  $T_{\text{max}} = 0.752$  3 standard reflections  
(expected range = 0.566–0.671) every 97 reflections  
8124 measured reflections intensity decay: <2%

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.083$  H atoms treated by a mixture of  
 $wR(F^2) = 0.190$  independent and constrained  
 $S = 1.03$  refinement  
7797 reflections  $\Delta\rho_{\text{max}} = 0.65$  e Å<sup>-3</sup>  
550 parameters  $\Delta\rho_{\text{min}} = -0.65$  e Å<sup>-3</sup>  
239 restraints

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}2A-\text{H}2A\cdots\text{O}1B$	0.76 (3)	1.93 (3)	2.664 (3)	162 (3)
$\text{O}2B-\text{H}2B\cdots\text{O}1A$	0.90 (3)	1.80 (3)	2.673 (3)	164 (3)
$\text{N}2A-\text{H}2AA\cdots\text{O}13C^i$	0.91	2.52	3.134 (8)	126
$\text{N}2A-\text{H}2AA\cdots\text{O}12A^i$	0.91	2.54	3.303 (7)	142
$\text{N}2B-\text{H}2BA\cdots\text{O}21^{ii}$	0.91	2.31	3.130 (4)	149
$\text{O}1M-\text{H}1M\cdots\text{O}14C^{iii}$	0.82	2.06	2.791 (9)	149
$\text{O}1M-\text{H}1M\cdots\text{O}11B^{iii}$	0.82	2.17	2.976 (10)	168
$\text{O}1M-\text{H}1M\cdots\text{O}14A^{iii}$	0.82	2.20	2.968 (7)	155
$\text{O}1M-\text{H}1M\cdots\text{O}13D^{iii}$	0.82	2.41	3.095 (11)	141
$\text{O}1M-\text{H}1M\cdots\text{O}12D^{iii}$	0.82	2.49	3.159 (11)	139
$\text{O}1M-\text{H}1M\cdots\text{O}13A^{iii}$	0.82	2.65	3.266 (7)	133

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: IM2022).

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**supplementary materials**

*Acta Cryst.* (2007). E63, m2863-m2864 [ doi:10.1107/S1600536807053500 ]

**Bis(2-{1-[2-(2-hydroxyethylamino)ethylimino]propyl}phenolato)-1 $\kappa^4$ O,N,N',O';2 $\kappa^4$ O,N,N',O'-methanol-2 $\kappa$ O- $\mu$ -perchlorato-1:2 $\kappa^2$ O:O'-perchlorato-1 $\kappa$ O-dicopper(II)**

**R. J. Butcher and W. Towns**

**Comment**

The structure of the title compound, (I), is shown in Figure 1, bond lengths and angles are available as Supplementary Material.

Hydrogen bonds play a key role in interactions in biological structures, supramolecular chemistry, and crystal engineering (Plass *et al.*, 2001). As such they are also important to understand the properties of relevant magnetic materials (Cros *et al.*, 1987). In particular for some copper(II)-containing coordination compounds it has been shown that the variation of possible supramolecular interactions can substantially influence the magnetic properties of related coordination polymers (Swamy *et al.*, 2001). As part of a program involving molecular recognition through intermolecular hydrogen bonding interactions (Butcher & Towns, 2005), the title compound was synthesized from 2-hydroxypropiophenone, copper(II) perchlorate, and 2-(2-aminoethylamino)ethanol in the presence of base.

The title compound consists of two six-coordinate Jahn-Teller distorted copper(II) complex units with the tetradentate ligand, (*N*-(2-hydroxypropiophenimine)-*N'*-(2-hydroxyethyl)ethylenediamine, observed in a planar coordination mode. The complex units are axially connected by a mutually  $\mu, \mu'$  bridging perchlorate anion. For one copper center the other axial position is occupied by a terminal methanol while for the other copper center the axial position is occupied by a weakly coordinated perchlorate anion. The two Cu complexes are also linked by intramolecular O—H $\cdots$ O hydrogen bonding interactions. In addition, there are also intermolecular N—H $\cdots$ O hydrogen bond interactions.

**Experimental**

The title compound, C<sub>27</sub>H<sub>41</sub>Cl<sub>2</sub>Cu<sub>2</sub>N<sub>4</sub>O<sub>13</sub>, was obtained by refluxing 2-hydroxypropiophenone (0.30 g, 2 mmol), 2-(2-aminoethylamino)ethanol (0.20 g, 2 mmol), and copper(II) perchlorate hexa hydrate (0.74 g, 2 mmol) in 200 ml of methanol in the presence of app. 2 ml base (trimethylamine or 2,6-dimethylpiperidine) for 1 h. The product deposited on cooling the solution. Suitable crystals were grown from a methanolic solution.

**Refinement**

The bridging perchlorate is disordered such that O24 is unique and the remaining O atoms are disordered over two conformations with occupancy factors of 0.63 (1) and 0.37 (1), respectively. The terminal perchlorate anion is disordered over three positions with multiplicities of 0.39 (4), 0.33 (3) and 0.28 (3). The thermal parameters of one of the perchlorate O atoms (O14D) did not behave well and thus were fixed. The H atoms were idealized with an N—H distance of 0.91 and C—H distances of 0.93 (aromatic C—H), 0.96 (CH<sub>3</sub>), and 0.97 (CH<sub>2</sub>) Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for the CH<sub>2</sub> groups and  $(1.5U_{\text{eq}}(\text{C}))$  for the CH<sub>3</sub> protons). The H atoms attached to O atoms were refined isotropically.

## Figures

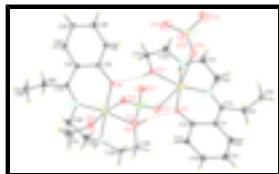


Fig. 1. The title compound with numbering scheme used. Hydrogen bonding interactions shown as dotted lines. Ellipsoids are drawn at the 20% probability level.

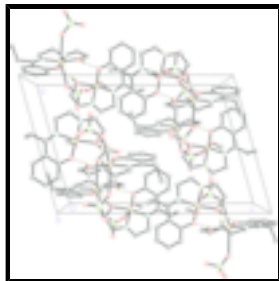


Fig. 2. The packing arrangement viewed down the *b* axis showing the intramolecular O—H...O and intermolecular N—H...O hydrogen bond interactions (dashed bonds).

**Bis(2-{1-[2-(2-hydroxyethylamino)ethylimino]propyl}phenolato)- 1κ<sup>4</sup>O,N,N',O';2κ<sup>4</sup>O,N,N',O'-methanol-2κO-μ-perchlorato-1:2κ<sup>2</sup>O:O'- perchlorato-1κO-dicopper(II)**

### Crystal data

[Cu <sub>2</sub> (C <sub>13</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> (C <sub>1</sub> H <sub>4</sub> O <sub>1</sub> )]	$F_{000} = 1712$
$M_r = 828.63$	$D_x = 1.618 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 13.405 (4) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 13.154 (5) \text{ \AA}$	Cell parameters from 30 reflections
$c = 20.019 (6) \text{ \AA}$	$\theta = 2.1\text{--}12.5^\circ$
$\beta = 105.52 (3)^\circ$	$\mu = 1.48 \text{ mm}^{-1}$
$V = 3401.4 (18) \text{ \AA}^3$	$T = 293 (2) \text{ K}$
$Z = 4$	Prism, dark green
	$0.45 \times 0.40 \times 0.27 \text{ mm}$

### Data collection

Bruker P4 diffractometer	4119 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.048$
Monochromator: graphite	$\theta_{\text{max}} = 27.5^\circ$
$T = 293(2) \text{ K}$	$\theta_{\text{min}} = 2.1^\circ$
2 $\theta/\omega$ scans	$h = -17 \rightarrow 0$
Absorption correction: empirical (using intensity measurements)	$k = -17 \rightarrow 0$
$\psi$ scans (North et al., 1968)	$l = -25 \rightarrow 26$
$T_{\text{min}} = 0.634$ , $T_{\text{max}} = 0.752$	3 standard reflections
8124 measured reflections	every 97 reflections
7797 independent reflections	

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.083$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.189$	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 9.8043P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
7797 reflections	$(\Delta/\sigma)_{\max} = 0.008$
550 parameters	$\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$
239 restraints	$\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	0.14849 (3)	0.51255 (3)	0.190520 (19)	0.04693 (11)	
Cu2	-0.02884 (3)	0.30996 (3)	0.328905 (18)	0.03873 (10)	
Cl1	0.45541 (7)	0.45505 (7)	0.29502 (6)	0.0708 (3)	
Cl2	-0.10543 (7)	0.57528 (6)	0.23851 (5)	0.0544 (3)	
O1M	0.0105 (2)	0.1247 (2)	0.34752 (14)	0.0858 (10)	
H1M	0.0106	0.1032	0.3091	0.103*	
O1A	0.10619 (15)	0.38175 (15)	0.16018 (9)	0.0418 (6)	
O2A	0.16987 (15)	0.48768 (16)	0.29101 (10)	0.0432 (6)	
H2A	0.142 (2)	0.447 (2)	0.3062 (15)	0.052*	
O1B	0.10558 (14)	0.35433 (16)	0.37063 (9)	0.0372 (6)	
O2B	-0.00764 (15)	0.29067 (17)	0.23388 (9)	0.0460 (6)	
H2B	0.040 (2)	0.313 (2)	0.2135 (15)	0.055*	
O11A	0.4335 (5)	0.4950 (5)	0.3564 (3)	0.110 (2)	0.4302 (1)
O12A	0.4813 (5)	0.3511 (4)	0.3035 (4)	0.108 (2)	0.4302 (1)
O13A	0.3707 (4)	0.4721 (5)	0.2345 (3)	0.090 (2)	0.4302 (1)
O14A	0.5437 (4)	0.5078 (5)	0.2841 (3)	0.118 (3)	0.4302 (1)

## supplementary materials

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O11B	0.4580 (7)	0.5628 (4)	0.2883 (4)	0.082 (3)	0.2496 (1)
O12B	0.4345 (7)	0.4296 (8)	0.3600 (3)	0.136 (4)	0.2496 (1)
O13B	0.5500 (4)	0.4112 (7)	0.2921 (5)	0.137 (3)	0.2496 (1)
O14B	0.3712 (5)	0.4153 (6)	0.2394 (4)	0.088 (3)	0.2496 (1)
O11C	0.5673 (4)	0.4637 (8)	0.3148 (5)	0.067 (3)	0.1858 (1)
O12C	0.4244 (6)	0.4529 (8)	0.3596 (3)	0.075 (3)	0.1858 (1)
O13C	0.4289 (8)	0.3609 (5)	0.2602 (4)	0.072 (3)	0.1858 (1)
O14C	0.4101 (7)	0.5390 (5)	0.2551 (4)	0.060 (3)	0.1858 (1)
O11D	0.4156 (6)	0.3574 (4)	0.3011 (5)	0.036 (3)	0.1345 (1)
O12D	0.5407 (5)	0.4480 (9)	0.2633 (4)	0.091 (4)	0.1345 (1)
O13D	0.3780 (6)	0.5186 (6)	0.2502 (5)	0.074 (4)	0.1345 (1)
O14D	0.4908 (10)	0.5026 (7)	0.3613 (3)	0.100*	0.1345 (1)
O21	-0.2137 (2)	0.5690 (2)	0.20947 (17)	0.0988 (10)	
O22	-0.0547 (2)	0.5460 (3)	0.18836 (15)	0.0986 (10)	
O23	-0.0772 (3)	0.6730 (2)	0.26572 (18)	0.1055 (11)	
O24	-0.0725 (2)	0.5066 (2)	0.29527 (14)	0.0783 (9)	
N1A	0.1606 (2)	0.5596 (2)	0.10104 (13)	0.0464 (8)	
N2A	0.1778 (3)	0.6545 (2)	0.22188 (14)	0.0706 (11)	
H2AA	0.1132	0.6819	0.2122	0.085*	
N1B	-0.07766 (18)	0.33053 (19)	0.41155 (12)	0.0403 (7)	
N2B	-0.17316 (18)	0.2742 (2)	0.28020 (13)	0.0473 (8)	
H2BA	-0.1802	0.2062	0.2860	0.057*	
C1M	-0.0237 (4)	0.0509 (4)	0.3833 (3)	0.116 (2)	
H1MA	0.0345	0.0147	0.4117	0.174*	
H1MB	-0.0672	0.0046	0.3513	0.174*	
H1MC	-0.0625	0.0811	0.4121	0.174*	
C1A	0.1222 (2)	0.3993 (2)	0.04164 (15)	0.0399 (9)	
C2A	0.1038 (2)	0.3433 (2)	0.09920 (15)	0.0402 (9)	
C3A	0.0778 (2)	0.2396 (3)	0.08817 (16)	0.0444 (10)	
H3AA	0.0639	0.2026	0.1243	0.053*	
C4A	0.0720 (2)	0.1905 (3)	0.02661 (18)	0.0588 (11)	
H4AA	0.0549	0.1219	0.0215	0.071*	
C5A	0.0921 (3)	0.2448 (3)	-0.02768 (18)	0.0679 (12)	
H5AA	0.0896	0.2124	-0.0694	0.082*	
C6A	0.1154 (3)	0.3452 (3)	-0.02011 (17)	0.0565 (11)	
H6AA	0.1275	0.3800	-0.0576	0.068*	
C7A	0.1448 (2)	0.5079 (3)	0.04489 (14)	0.0431 (9)	
C8A	0.1536 (3)	0.5602 (3)	-0.02135 (15)	0.0548 (11)	
H8AA	0.1071	0.5274	-0.0610	0.066*	
H8AB	0.1323	0.6306	-0.0208	0.066*	
C9A	0.2628 (3)	0.5564 (4)	-0.0292 (2)	0.0911 (16)	
H9AA	0.2634	0.5833	-0.0737	0.137*	
H9AB	0.2865	0.4873	-0.0257	0.137*	
H9AC	0.3076	0.5963	0.0067	0.137*	
C10A	0.1841 (3)	0.6685 (3)	0.10308 (18)	0.0662 (12)	
H10A	0.2373	0.6812	0.0794	0.079*	
H10B	0.1226	0.7061	0.0793	0.079*	
C11A	0.2199 (3)	0.7033 (3)	0.17473 (19)	0.0792 (14)	
H11A	0.2946	0.6955	0.1898	0.095*	

H11D	0.2050	0.7754	0.1759	0.095*
C12A	0.2094 (4)	0.6612 (3)	0.29207 (18)	0.0741 (15)
H12A	0.1813	0.7235	0.3055	0.089*
H12D	0.2842	0.6680	0.3054	0.089*
C13A	0.1833 (3)	0.5803 (2)	0.33157 (16)	0.0531 (11)
H13A	0.1199	0.5964	0.3438	0.064*
H13B	0.2380	0.5712	0.3741	0.064*
C1B	0.0881 (2)	0.3723 (2)	0.48796 (14)	0.0398 (9)
C2B	0.1461 (2)	0.3745 (2)	0.43768 (14)	0.0362 (8)
C3B	0.2504 (2)	0.4007 (2)	0.45846 (15)	0.0419 (9)
H3BA	0.2877	0.4020	0.4254	0.050*
C4B	0.3004 (3)	0.4246 (3)	0.52616 (16)	0.0521 (11)
H4BA	0.3704	0.4415	0.5386	0.063*
C5B	0.2455 (3)	0.4233 (3)	0.57492 (17)	0.0577 (12)
H5BA	0.2780	0.4404	0.6207	0.069*
C6B	0.1436 (3)	0.3972 (3)	0.55661 (16)	0.0542 (11)
H6BA	0.1086	0.3956	0.5909	0.065*
C7B	-0.0219 (2)	0.3495 (2)	0.47347 (14)	0.0428 (9)
C8B	-0.0726 (3)	0.3432 (3)	0.53342 (16)	0.0662 (12)
H8BA	-0.0418	0.3934	0.5684	0.079*
H8BB	-0.1459	0.3579	0.5165	0.079*
C9B	-0.0575 (4)	0.2373 (3)	0.5654 (2)	0.0963 (16)
H9BA	-0.0915	0.2332	0.6019	0.144*
H9BB	0.0151	0.2242	0.5840	0.144*
H9BC	-0.0867	0.1876	0.5305	0.144*
C10B	-0.1908 (2)	0.3119 (3)	0.39431 (17)	0.0557 (10)
H10C	-0.2226	0.3591	0.4196	0.067*
H10D	-0.2038	0.2433	0.4078	0.067*
C11B	-0.2366 (2)	0.3253 (3)	0.3185 (2)	0.0724 (13)
H11B	-0.3061	0.2974	0.3053	0.087*
H11C	-0.2410	0.3972	0.3072	0.087*
C12B	-0.1916 (3)	0.2919 (3)	0.20665 (17)	0.0608 (12)
H12B	-0.2049	0.3636	0.1967	0.073*
H12C	-0.2521	0.2539	0.1815	0.073*
C13B	-0.1007 (3)	0.2598 (3)	0.18377 (17)	0.0617 (12)
H13C	-0.1012	0.1865	0.1784	0.074*
H13D	-0.1034	0.2903	0.1392	0.074*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0725 (2)	0.0371 (2)	0.03671 (17)	-0.0156 (2)	0.02405 (16)	-0.00140 (17)
Cu2	0.03875 (16)	0.0461 (2)	0.03576 (16)	-0.00538 (18)	0.01762 (13)	-0.00192 (17)
Cl1	0.0591 (5)	0.0495 (5)	0.1053 (7)	0.0015 (5)	0.0246 (5)	0.0053 (5)
Cl2	0.0473 (4)	0.0415 (4)	0.0707 (5)	-0.0018 (4)	0.0093 (4)	0.0003 (4)
O1M	0.1241 (19)	0.0559 (16)	0.0965 (17)	-0.0002 (16)	0.0627 (14)	0.0035 (14)
O1A	0.0614 (12)	0.0350 (11)	0.0346 (9)	-0.0068 (10)	0.0227 (8)	-0.0032 (9)
O2A	0.0575 (11)	0.0393 (11)	0.0381 (10)	-0.0060 (10)	0.0222 (9)	0.0004 (9)



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O1B	0.0382 (10)	0.0459 (12)	0.0318 (9)	-0.0055 (9)	0.0167 (8)	-0.0071 (9)
O2B	0.0516 (11)	0.0587 (13)	0.0315 (9)	-0.0222 (11)	0.0174 (8)	-0.0062 (10)
O11A	0.105 (4)	0.115 (4)	0.113 (4)	0.015 (3)	0.035 (3)	-0.030 (3)
O12A	0.112 (4)	0.081 (4)	0.126 (4)	0.012 (3)	0.025 (3)	0.015 (3)
O13A	0.085 (3)	0.102 (4)	0.082 (3)	0.022 (3)	0.019 (3)	-0.002 (3)
O14A	0.113 (4)	0.116 (4)	0.125 (4)	-0.032 (3)	0.030 (3)	0.023 (3)
O11B	0.089 (5)	0.065 (4)	0.088 (5)	0.000 (4)	0.016 (4)	-0.006 (4)
O12B	0.141 (5)	0.138 (5)	0.131 (5)	-0.005 (4)	0.041 (4)	0.018 (4)
O13B	0.133 (5)	0.131 (5)	0.146 (5)	0.016 (4)	0.036 (4)	-0.004 (4)
O14B	0.087 (5)	0.079 (5)	0.095 (5)	-0.002 (4)	0.020 (4)	-0.004 (4)
O11C	0.058 (5)	0.069 (5)	0.077 (5)	0.005 (4)	0.023 (4)	-0.005 (4)
O12C	0.082 (5)	0.073 (5)	0.072 (5)	0.000 (4)	0.026 (4)	0.013 (4)
O13C	0.074 (5)	0.063 (5)	0.071 (5)	-0.007 (4)	0.007 (4)	0.001 (4)
O14C	0.055 (5)	0.057 (5)	0.066 (5)	0.002 (4)	0.014 (4)	0.010 (4)
O11D	0.033 (5)	0.024 (5)	0.050 (5)	-0.013 (4)	0.007 (4)	-0.002 (4)
O12D	0.089 (6)	0.092 (6)	0.095 (6)	0.006 (5)	0.026 (4)	0.004 (5)
O13D	0.073 (5)	0.070 (6)	0.078 (6)	0.000 (4)	0.020 (4)	0.008 (4)
O21	0.0706 (15)	0.0900 (17)	0.1269 (19)	0.0030 (14)	0.0109 (14)	-0.0201 (15)
O22	0.0915 (16)	0.133 (2)	0.0777 (15)	-0.0004 (16)	0.0343 (12)	0.0057 (15)
O23	0.1000 (18)	0.0687 (16)	0.1237 (19)	-0.0029 (15)	-0.0117 (15)	-0.0020 (15)
O24	0.0874 (15)	0.0730 (15)	0.0777 (14)	-0.0033 (13)	0.0274 (12)	0.0100 (13)
N1A	0.0540 (14)	0.0445 (15)	0.0458 (13)	-0.0021 (13)	0.0220 (11)	0.0082 (12)
N2A	0.122 (2)	0.0462 (16)	0.0495 (15)	-0.0310 (17)	0.0331 (15)	-0.0081 (14)
N1B	0.0515 (13)	0.0386 (14)	0.0399 (11)	-0.0063 (12)	0.0278 (9)	-0.0013 (11)
N2B	0.0392 (13)	0.0548 (16)	0.0487 (14)	-0.0075 (13)	0.0134 (11)	-0.0017 (13)
C1M	0.120 (4)	0.103 (4)	0.121 (4)	-0.012 (3)	0.025 (3)	0.045 (3)
C1A	0.0329 (15)	0.0490 (18)	0.0368 (15)	0.0037 (15)	0.0077 (12)	-0.0028 (14)
C2A	0.0391 (15)	0.0409 (17)	0.0405 (15)	0.0076 (14)	0.0106 (13)	-0.0074 (14)
C3A	0.0429 (16)	0.0479 (19)	0.0426 (16)	0.0019 (16)	0.0115 (13)	-0.0069 (15)
C4A	0.0487 (18)	0.059 (2)	0.070 (2)	0.0056 (18)	0.0181 (16)	-0.0262 (18)
C5A	0.0584 (19)	0.097 (3)	0.0526 (18)	0.008 (2)	0.0218 (15)	-0.0315 (19)
C6A	0.0557 (19)	0.073 (2)	0.0441 (17)	0.0035 (19)	0.0195 (14)	-0.0078 (17)
C7A	0.0390 (15)	0.062 (2)	0.0297 (13)	0.0095 (16)	0.0125 (11)	0.0132 (15)
C8A	0.0609 (19)	0.068 (2)	0.0410 (15)	0.0100 (18)	0.0230 (14)	0.0196 (16)
C9A	0.075 (2)	0.139 (4)	0.070 (2)	0.010 (3)	0.0391 (18)	0.038 (3)
C10A	0.091 (2)	0.057 (2)	0.0603 (19)	-0.017 (2)	0.0355 (17)	0.0089 (18)
C11A	0.118 (3)	0.052 (2)	0.078 (2)	-0.034 (2)	0.044 (2)	0.0023 (19)
C12A	0.121 (3)	0.041 (2)	0.054 (2)	-0.012 (2)	0.014 (2)	-0.0045 (18)
C13A	0.071 (2)	0.0467 (19)	0.0437 (17)	-0.0119 (18)	0.0196 (15)	-0.0080 (16)
C1B	0.0644 (18)	0.0271 (15)	0.0313 (13)	0.0115 (14)	0.0184 (13)	0.0043 (12)
C2B	0.0465 (16)	0.0269 (14)	0.0338 (14)	0.0050 (14)	0.0083 (12)	0.0000 (12)
C3B	0.0469 (17)	0.0405 (17)	0.0383 (15)	0.0051 (15)	0.0111 (13)	-0.0036 (14)
C4B	0.055 (2)	0.0454 (19)	0.0463 (19)	0.0112 (17)	-0.0024 (17)	-0.0029 (16)
C5B	0.080 (2)	0.047 (2)	0.0351 (17)	0.0136 (19)	-0.0033 (17)	-0.0042 (16)
C6B	0.085 (2)	0.049 (2)	0.0320 (14)	0.0109 (19)	0.0229 (15)	0.0036 (15)
C7B	0.0684 (17)	0.0302 (15)	0.0410 (13)	0.0101 (15)	0.0339 (12)	-0.0004 (13)
C8B	0.095 (2)	0.072 (2)	0.0480 (16)	0.000 (2)	0.0467 (14)	-0.0044 (17)
C9B	0.164 (4)	0.070 (3)	0.075 (2)	-0.017 (3)	0.067 (2)	0.013 (2)
C10B	0.0549 (17)	0.055 (2)	0.0687 (18)	-0.0128 (17)	0.0363 (14)	-0.0070 (17)

C11B	0.0366 (16)	0.085 (3)	0.102 (3)	-0.0170 (19)	0.0299 (16)	-0.035 (2)
C12B	0.053 (2)	0.070 (2)	0.055 (2)	-0.010 (2)	0.0057 (17)	-0.0086 (19)
C13B	0.063 (2)	0.077 (2)	0.0428 (18)	-0.025 (2)	0.0110 (16)	-0.0116 (19)

*Geometric parameters (Å, °)*

Cu1—O1A	1.862 (2)	C3A—C4A	1.375 (5)
Cu1—N1A	1.943 (3)	C3A—H3AA	0.9300
Cu1—N2A	1.975 (3)	C4A—C5A	1.386 (5)
Cu1—O2A	1.982 (2)	C4A—H4AA	0.9300
Cu1—O22	2.748 (3)	C5A—C6A	1.356 (6)
Cu1—O13A	2.921 (5)	C5A—H5AA	0.9300
Cu2—O1B	1.8654 (19)	C6A—H6AA	0.9300
Cu2—N1B	1.954 (3)	C7A—C8A	1.526 (4)
Cu2—N2B	1.976 (2)	C8A—C9A	1.514 (5)
Cu2—O2B	2.013 (2)	C8A—H8AA	0.9700
Cu2—O1M	2.500 (3)	C8A—H8AB	0.9700
Cu2—O24	2.698 (3)	C9A—H9AA	0.9600
Cl1—O14C	1.403 (6)	C9A—H9AB	0.9600
Cl1—O13B	1.408 (7)	C9A—H9AC	0.9600
Cl1—O11D	1.409 (6)	C10A—C11A	1.459 (5)
Cl1—O12A	1.410 (5)	C10A—H10A	0.9700
Cl1—O13C	1.420 (6)	C10A—H10B	0.9700
Cl1—O11B	1.425 (5)	C11A—H11A	0.9700
Cl1—O14D	1.428 (7)	C11A—H11D	0.9700
Cl1—O11A	1.438 (6)	C12A—C13A	1.424 (5)
Cl1—O13A	1.439 (5)	C12A—H12A	0.9700
Cl1—O14A	1.439 (6)	C12A—H12D	0.9700
Cl1—O12B	1.443 (7)	C13A—H13A	0.9700
Cl1—O13D	1.443 (7)	C13A—H13B	0.9700
Cl2—O23	1.408 (3)	C1B—C6B	1.415 (4)
Cl2—O22	1.409 (3)	C1B—C2B	1.427 (5)
Cl2—O21	1.414 (3)	C1B—C7B	1.457 (4)
Cl2—O24	1.426 (3)	C2B—C3B	1.391 (4)
O1M—C1M	1.357 (6)	C3B—C4B	1.378 (4)
O1M—H1M	0.8200	C3B—H3BA	0.9300
O1A—C2A	1.314 (4)	C4B—C5B	1.371 (5)
O2A—C13A	1.448 (4)	C4B—H4BA	0.9300
O2A—H2A	0.76 (3)	C5B—C6B	1.360 (5)
O1B—C2B	1.333 (3)	C5B—H5BA	0.9300
O2B—C13B	1.435 (4)	C6B—H6BA	0.9300
O2B—H2B	0.90 (3)	C7B—C8B	1.531 (5)
N1A—C7A	1.282 (4)	C8B—C9B	1.524 (6)
N1A—C10A	1.465 (4)	C8B—H8BA	0.9700
N2A—C12A	1.358 (4)	C8B—H8BB	0.9700
N2A—C11A	1.381 (5)	C9B—H9BA	0.9600
N2A—H2AA	0.9100	C9B—H9BB	0.9600
N1B—C7B	1.289 (3)	C9B—H9BC	0.9600
N1B—C10B	1.483 (4)	C10B—C11B	1.488 (5)

## supplementary materials

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N2B—C12B	1.445 (4)	C10B—H10C	0.9700
N2B—C11B	1.453 (5)	C10B—H10D	0.9700
N2B—H2BA	0.9100	C11B—H11B	0.9700
C1M—H1MA	0.9600	C11B—H11C	0.9700
C1M—H1MB	0.9600	C12B—C13B	1.474 (5)
C1M—H1MC	0.9600	C12B—H12B	0.9700
C1A—C6A	1.408 (5)	C12B—H12C	0.9700
C1A—C2A	1.444 (4)	C13B—H13C	0.9700
C1A—C7A	1.458 (5)	C13B—H13D	0.9700
C2A—C3A	1.411 (4)		
O1A—Cu1—N1A	94.99 (10)	C10B—N1B—Cu2	109.48 (18)
O1A—Cu1—N2A	173.93 (13)	C12B—N2B—C11B	119.9 (3)
N1A—Cu1—N2A	86.18 (12)	C12B—N2B—Cu2	110.0 (2)
O1A—Cu1—O2A	97.32 (9)	C11B—N2B—Cu2	105.29 (19)
N1A—Cu1—O2A	164.47 (10)	C12B—N2B—H2BA	107.0
N2A—Cu1—O2A	82.59 (10)	C11B—N2B—H2BA	107.0
O1A—Cu1—O22	85.91 (10)	Cu2—N2B—H2BA	107.0
N1A—Cu1—O22	105.17 (10)	O1M—C1M—H1MA	109.5
N2A—Cu1—O22	88.04 (13)	O1M—C1M—H1MB	109.5
O2A—Cu1—O22	85.17 (9)	H1MA—C1M—H1MB	109.5
O1A—Cu1—O13A	97.29 (14)	O1M—C1M—H1MC	109.5
N1A—Cu1—O13A	90.34 (14)	H1MA—C1M—H1MC	109.5
N2A—Cu1—O13A	88.65 (16)	H1MB—C1M—H1MC	109.5
O2A—Cu1—O13A	78.76 (13)	C6A—C1A—C2A	117.2 (3)
O22—Cu1—O13A	163.88 (13)	C6A—C1A—C7A	119.9 (3)
O1B—Cu2—N1B	94.58 (9)	C2A—C1A—C7A	122.8 (3)
O1B—Cu2—N2B	175.01 (10)	O1A—C2A—C3A	117.5 (3)
N1B—Cu2—N2B	86.86 (11)	O1A—C2A—C1A	125.3 (3)
O1B—Cu2—O2B	95.67 (9)	C3A—C2A—C1A	117.2 (3)
N1B—Cu2—O2B	168.94 (9)	C4A—C3A—C2A	123.1 (3)
N2B—Cu2—O2B	82.58 (10)	C4A—C3A—H3AA	118.4
O1B—Cu2—O1M	95.65 (9)	C2A—C3A—H3AA	118.4
N1B—Cu2—O1M	96.53 (10)	C3A—C4A—C5A	119.0 (3)
N2B—Cu2—O1M	88.92 (10)	C3A—C4A—H4AA	120.5
O2B—Cu2—O1M	86.59 (9)	C5A—C4A—H4AA	120.5
O1B—Cu2—O24	86.03 (9)	C6A—C5A—C4A	120.1 (3)
N1B—Cu2—O24	88.80 (10)	C6A—C5A—H5AA	119.9
N2B—Cu2—O24	89.23 (10)	C4A—C5A—H5AA	119.9
O2B—Cu2—O24	87.77 (9)	C5A—C6A—C1A	123.3 (3)
O1M—Cu2—O24	174.25 (9)	C5A—C6A—H6AA	118.3
O14C—Cl1—O13B	123.8 (6)	C1A—C6A—H6AA	118.3
O14C—Cl1—O11D	130.6 (5)	N1A—C7A—C1A	122.9 (3)
O13B—Cl1—O11D	89.8 (5)	N1A—C7A—C8A	119.3 (3)
O14C—Cl1—O12A	152.5 (4)	C1A—C7A—C8A	117.8 (3)
O13B—Cl1—O12A	54.0 (5)	C9A—C8A—C7A	112.2 (3)
O11D—Cl1—O12A	36.1 (4)	C9A—C8A—H8AA	109.2
O14C—Cl1—O13C	113.2 (4)	C7A—C8A—H8AA	109.2
O13B—Cl1—O13C	74.4 (5)	C9A—C8A—H8AB	109.2
O11D—Cl1—O13C	36.5 (6)	C7A—C8A—H8AB	109.2

O12A—C11—O13C	40.0 (4)	H8AA—C8A—H8AB	107.9
O14C—C11—O11B	35.0 (4)	C8A—C9A—H9AA	109.5
O13B—C11—O11B	111.0 (5)	C8A—C9A—H9AB	109.5
O11D—C11—O11B	159.2 (5)	H9AA—C9A—H9AB	109.5
O12A—C11—O11B	164.7 (5)	C8A—C9A—H9AC	109.5
O13C—C11—O11B	146.2 (5)	H9AA—C9A—H9AC	109.5
O14C—C11—O14D	99.8 (5)	H9AB—C9A—H9AC	109.5
O13B—C11—O14D	98.0 (6)	C11A—C10A—N1A	110.2 (3)
O11D—C11—O14D	111.0 (6)	C11A—C10A—H10A	109.6
O12A—C11—O14D	107.7 (5)	N1A—C10A—H10A	109.6
O13C—C11—O14D	144.7 (5)	C11A—C10A—H10B	109.6
O11B—C11—O14D	69.0 (5)	N1A—C10A—H10B	109.6
O14C—C11—O11A	92.5 (4)	H10A—C10A—H10B	108.1
O13B—C11—O11A	125.3 (5)	N2A—C11A—C10A	116.0 (3)
O11D—C11—O11A	95.2 (5)	N2A—C11A—H11A	108.3
O12A—C11—O11A	110.6 (4)	C10A—C11A—H11A	108.3
O13C—C11—O11A	131.1 (5)	N2A—C11A—H11D	108.3
O11B—C11—O11A	74.5 (5)	C10A—C11A—H11D	108.3
O14D—C11—O11A	30.5 (6)	H11A—C11A—H11D	107.4
O14C—C11—O13A	43.4 (4)	N2A—C12A—C13A	118.1 (3)
O13B—C11—O13A	123.0 (5)	N2A—C12A—H12A	107.8
O11D—C11—O13A	89.1 (4)	C13A—C12A—H12A	107.8
O12A—C11—O13A	111.4 (4)	N2A—C12A—H12D	107.8
O13C—C11—O13A	71.6 (4)	C13A—C12A—H12D	107.8
O11B—C11—O13A	78.5 (4)	H12A—C12A—H12D	107.1
O14D—C11—O13A	134.8 (5)	C12A—C13A—O2A	109.2 (3)
O11A—C11—O13A	111.5 (3)	C12A—C13A—H13A	109.8
O14C—C11—O14A	77.4 (4)	O2A—C13A—H13A	109.8
O13B—C11—O14A	53.5 (5)	C12A—C13A—H13B	109.8
O11D—C11—O14A	143.1 (5)	O2A—C13A—H13B	109.8
O12A—C11—O14A	107.5 (4)	H13A—C13A—H13B	108.3
O13C—C11—O14A	117.0 (5)	C6B—C1B—C2B	115.9 (3)
O11B—C11—O14A	57.6 (5)	C6B—C1B—C7B	118.8 (3)
O14D—C11—O14A	81.3 (6)	C2B—C1B—C7B	125.3 (2)
O11A—C11—O14A	108.6 (4)	O1B—C2B—C3B	117.2 (3)
O13A—C11—O14A	107.0 (4)	O1B—C2B—C1B	123.7 (3)
O14C—C11—O12B	122.6 (6)	C3B—C2B—C1B	119.2 (3)
O13B—C11—O12B	109.7 (5)	C4B—C3B—C2B	122.4 (3)
O11D—C11—O12B	62.6 (6)	C4B—C3B—H3BA	118.8
O12A—C11—O12B	76.5 (5)	C2B—C3B—H3BA	118.8
O13C—C11—O12B	99.0 (6)	C5B—C4B—C3B	119.0 (3)
O11B—C11—O12B	109.4 (5)	C5B—C4B—H4BA	120.5
O14D—C11—O12B	50.2 (6)	C3B—C4B—H4BA	120.5
O11A—C11—O12B	34.9 (5)	C6B—C5B—C4B	120.2 (3)
O13A—C11—O12B	119.7 (4)	C6B—C5B—H5BA	119.9
O14A—C11—O12B	128.0 (4)	C4B—C5B—H5BA	119.9
O14C—C11—O13D	20.0 (5)	C5B—C6B—C1B	123.3 (3)
O13B—C11—O13D	135.8 (6)	C5B—C6B—H6BA	118.4
O11D—C11—O13D	110.9 (5)	C1B—C6B—H6BA	118.4

## supplementary materials

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O12A—C11—O13D	138.5 (4)	N1B—C7B—C1B	121.8 (3)
O13C—C11—O13D	99.0 (5)	N1B—C7B—C8B	118.6 (3)
O11B—C11—O13D	52.9 (5)	C1B—C7B—C8B	119.5 (2)
O14D—C11—O13D	109.2 (6)	C9B—C8B—C7B	110.0 (3)
O11A—C11—O13D	92.4 (5)	C9B—C8B—H8BA	109.7
O13A—C11—O13D	27.4 (4)	C7B—C8B—H8BA	109.7
O14A—C11—O13D	96.3 (5)	C9B—C8B—H8BB	109.7
O12B—C11—O13D	114.5 (6)	C7B—C8B—H8BB	109.7
O23—C12—O22	113.2 (2)	H8BA—C8B—H8BB	108.2
O23—C12—O21	110.6 (2)	C8B—C9B—H9BA	109.5
O22—C12—O21	109.22 (19)	C8B—C9B—H9BB	109.5
O23—C12—O24	106.04 (18)	H9BA—C9B—H9BB	109.5
O22—C12—O24	106.80 (19)	C8B—C9B—H9BC	109.5
O21—C12—O24	110.83 (19)	H9BA—C9B—H9BC	109.5
C1M—O1M—Cu2	133.6 (3)	H9BB—C9B—H9BC	109.5
C1M—O1M—H1M	109.5	N1B—C10B—C11B	109.6 (3)
Cu2—O1M—H1M	104.4	N1B—C10B—H10C	109.8
C2A—O1A—Cu1	126.1 (2)	C11B—C10B—H10C	109.8
C13A—O2A—Cu1	113.12 (17)	N1B—C10B—H10D	109.8
C13A—O2A—H2A	111 (2)	C11B—C10B—H10D	109.8
Cu1—O2A—H2A	125 (2)	H10C—C10B—H10D	108.2
C2B—O1B—Cu2	126.70 (19)	N2B—C11B—C10B	110.1 (3)
C13B—O2B—Cu2	112.3 (2)	N2B—C11B—H11B	109.6
C13B—O2B—H2B	111.7 (17)	C10B—C11B—H11B	109.6
Cu2—O2B—H2B	133.3 (18)	N2B—C11B—H11C	109.6
C11—O13A—Cu1	142.5 (3)	C10B—C11B—H11C	109.6
C12—O22—Cu1	134.28 (16)	H11B—C11B—H11C	108.2
C12—O24—Cu2	143.76 (17)	N2B—C12B—C13B	109.9 (3)
C7A—N1A—C10A	121.8 (3)	N2B—C12B—H12B	109.7
C7A—N1A—Cu1	127.2 (2)	C13B—C12B—H12B	109.7
C10A—N1A—Cu1	110.9 (2)	N2B—C12B—H12C	109.7
C12A—N2A—C11A	127.3 (3)	C13B—C12B—H12C	109.7
C12A—N2A—Cu1	111.8 (2)	H12B—C12B—H12C	108.2
C11A—N2A—Cu1	107.8 (2)	O2B—C13B—C12B	109.8 (3)
C12A—N2A—H2AA	102.1	O2B—C13B—H13C	109.7
C11A—N2A—H2AA	102.1	C12B—C13B—H13C	109.7
Cu1—N2A—H2AA	102.1	O2B—C13B—H13D	109.7
C7B—N1B—C10B	123.3 (3)	C12B—C13B—H13D	109.7
C7B—N1B—Cu2	127.0 (2)	H13C—C13B—H13D	108.2
O1B—Cu2—O1M—C1M	118.3 (4)	O24—Cu2—N1B—C7B	-97.1 (3)
N1B—Cu2—O1M—C1M	23.0 (4)	O1B—Cu2—N1B—C10B	174.0 (2)
N2B—Cu2—O1M—C1M	-63.7 (4)	N2B—Cu2—N1B—C10B	-1.3 (2)
O2B—Cu2—O1M—C1M	-146.3 (4)	O2B—Cu2—N1B—C10B	16.1 (6)
O24—Cu2—O1M—C1M	-135.0 (9)	O1M—Cu2—N1B—C10B	-89.8 (2)
N1A—Cu1—O1A—C2A	7.8 (2)	O24—Cu2—N1B—C10B	88.0 (2)
N2A—Cu1—O1A—C2A	108.6 (10)	O1B—Cu2—N2B—C12B	48.7 (13)
O2A—Cu1—O1A—C2A	-162.7 (2)	N1B—Cu2—N2B—C12B	155.6 (2)
O22—Cu1—O1A—C2A	112.7 (2)	O2B—Cu2—N2B—C12B	-21.1 (2)
O13A—Cu1—O1A—C2A	-83.2 (2)	O1M—Cu2—N2B—C12B	-107.8 (2)

O1A—Cu1—O2A—C13A	-167.8 (2)	O24—Cu2—N2B—C12B	66.8 (2)
N1A—Cu1—O2A—C13A	50.0 (5)	O1B—Cu2—N2B—C11B	-81.8 (12)
N2A—Cu1—O2A—C13A	6.1 (2)	N1B—Cu2—N2B—C11B	25.1 (2)
O22—Cu1—O2A—C13A	-82.6 (2)	O2B—Cu2—N2B—C11B	-151.6 (2)
O13A—Cu1—O2A—C13A	96.2 (2)	O1M—Cu2—N2B—C11B	121.7 (2)
N1B—Cu2—O1B—C2B	9.1 (2)	O24—Cu2—N2B—C11B	-63.7 (2)
N2B—Cu2—O1B—C2B	115.7 (12)	Cu1—O1A—C2A—C3A	174.6 (2)
O2B—Cu2—O1B—C2B	-175.1 (2)	Cu1—O1A—C2A—C1A	-7.6 (4)
O1M—Cu2—O1B—C2B	-88.0 (2)	C6A—C1A—C2A—O1A	-179.5 (3)
O24—Cu2—O1B—C2B	97.5 (2)	C7A—C1A—C2A—O1A	-0.9 (5)
O1B—Cu2—O2B—C13B	-177.1 (2)	C6A—C1A—C2A—C3A	-1.6 (4)
N1B—Cu2—O2B—C13B	-19.3 (6)	C7A—C1A—C2A—C3A	177.0 (3)
N2B—Cu2—O2B—C13B	-1.8 (2)	O1A—C2A—C3A—C4A	179.6 (3)
O1M—Cu2—O2B—C13B	87.5 (2)	C1A—C2A—C3A—C4A	1.6 (4)
O24—Cu2—O2B—C13B	-91.3 (2)	C2A—C3A—C4A—C5A	-0.3 (5)
O14C—Cl1—O13A—Cu1	-91.4 (9)	C3A—C4A—C5A—C6A	-1.0 (5)
O13B—Cl1—O13A—Cu1	162.5 (6)	C4A—C5A—C6A—C1A	1.0 (5)
O11D—Cl1—O13A—Cu1	73.4 (7)	C2A—C1A—C6A—C5A	0.4 (5)
O12A—Cl1—O13A—Cu1	102.4 (6)	C7A—C1A—C6A—C5A	-178.2 (3)
O13C—Cl1—O13A—Cu1	106.1 (7)	C10A—N1A—C7A—C1A	179.4 (3)
O11B—Cl1—O13A—Cu1	-89.8 (7)	Cu1—N1A—C7A—C1A	-5.2 (4)
O14D—Cl1—O13A—Cu1	-45.8 (10)	C10A—N1A—C7A—C8A	1.8 (5)
O11A—Cl1—O13A—Cu1	-21.8 (7)	Cu1—N1A—C7A—C8A	177.2 (2)
O14A—Cl1—O13A—Cu1	-140.4 (6)	C6A—C1A—C7A—N1A	-173.9 (3)
O12B—Cl1—O13A—Cu1	16.0 (9)	C2A—C1A—C7A—N1A	7.5 (5)
O13D—Cl1—O13A—Cu1	-70.3 (11)	C6A—C1A—C7A—C8A	3.7 (4)
O1A—Cu1—O13A—Cl1	-102.7 (6)	C2A—C1A—C7A—C8A	-174.8 (3)
N1A—Cu1—O13A—Cl1	162.2 (6)	N1A—C7A—C8A—C9A	89.0 (4)
N2A—Cu1—O13A—Cl1	76.1 (6)	C1A—C7A—C8A—C9A	-88.7 (4)
O2A—Cu1—O13A—Cl1	-6.7 (6)	C7A—N1A—C10A—C11A	-168.0 (3)
O22—Cu1—O13A—Cl1	-2.1 (11)	Cu1—N1A—C10A—C11A	15.9 (4)
O23—Cl2—O22—Cu1	63.1 (3)	C12A—N2A—C11A—C10A	168.8 (4)
O21—Cl2—O22—Cu1	-173.2 (2)	Cu1—N2A—C11A—C10A	31.7 (4)
O24—Cl2—O22—Cu1	-53.3 (3)	N1A—C10A—C11A—N2A	-32.4 (5)
O1A—Cu1—O22—Cl2	121.4 (3)	C11A—N2A—C12A—C13A	-157.4 (4)
N1A—Cu1—O22—Cl2	-144.5 (3)	Cu1—N2A—C12A—C13A	-21.6 (5)
N2A—Cu1—O22—Cl2	-59.0 (3)	N2A—C12A—C13A—O2A	26.1 (5)
O2A—Cu1—O22—Cl2	23.7 (3)	Cu1—O2A—C13A—C12A	-17.9 (3)
O13A—Cu1—O22—Cl2	19.2 (7)	Cu2—O1B—C2B—C3B	176.1 (2)
O23—Cl2—O24—Cu2	-161.3 (3)	Cu2—O1B—C2B—C1B	-5.1 (4)
O22—Cl2—O24—Cu2	-40.3 (3)	C6B—C1B—C2B—O1B	-179.1 (3)
O21—Cl2—O24—Cu2	78.6 (3)	C7B—C1B—C2B—O1B	-0.9 (5)
O1B—Cu2—O24—Cl2	117.3 (3)	C6B—C1B—C2B—C3B	-0.3 (4)
N1B—Cu2—O24—Cl2	-148.0 (3)	C7B—C1B—C2B—C3B	177.9 (3)
N2B—Cu2—O24—Cl2	-61.2 (3)	O1B—C2B—C3B—C4B	179.0 (3)
O2B—Cu2—O24—Cl2	21.4 (3)	C1B—C2B—C3B—C4B	0.1 (5)
O1M—Cu2—O24—Cl2	10.1 (11)	C2B—C3B—C4B—C5B	-0.4 (5)
O1A—Cu1—N1A—C7A	-1.6 (3)	C3B—C4B—C5B—C6B	1.0 (5)
N2A—Cu1—N1A—C7A	-175.6 (3)	C4B—C5B—C6B—C1B	-1.3 (5)

## supplementary materials

O2A—Cu1—N1A—C7A	140.8 (3)	C2B—C1B—C6B—C5B	0.9 (5)
O22—Cu1—N1A—C7A	-88.7 (3)	C7B—C1B—C6B—C5B	-177.4 (3)
O13A—Cu1—N1A—C7A	95.8 (3)	C10B—N1B—C7B—C1B	-177.0 (3)
O1A—Cu1—N1A—C10A	174.3 (2)	Cu2—N1B—C7B—C1B	8.8 (4)
N2A—Cu1—N1A—C10A	0.3 (2)	C10B—N1B—C7B—C8B	5.6 (4)
O2A—Cu1—N1A—C10A	-43.4 (5)	Cu2—N1B—C7B—C8B	-168.6 (2)
O22—Cu1—N1A—C10A	87.2 (2)	C6B—C1B—C7B—N1B	177.0 (3)
O13A—Cu1—N1A—C10A	-88.4 (3)	C2B—C1B—C7B—N1B	-1.2 (5)
O1A—Cu1—N2A—C12A	97.3 (10)	C6B—C1B—C7B—C8B	-5.7 (4)
N1A—Cu1—N2A—C12A	-161.4 (3)	C2B—C1B—C7B—C8B	176.1 (3)
O2A—Cu1—N2A—C12A	7.9 (3)	N1B—C7B—C8B—C9B	92.8 (4)
O22—Cu1—N2A—C12A	93.2 (3)	C1B—C7B—C8B—C9B	-84.6 (4)
O13A—Cu1—N2A—C12A	-71.0 (3)	C7B—N1B—C10B—C11B	162.0 (3)
O1A—Cu1—N2A—C11A	-118.3 (10)	Cu2—N1B—C10B—C11B	-22.8 (3)
N1A—Cu1—N2A—C11A	-17.1 (3)	C12B—N2B—C11B—C10B	-168.9 (3)
O2A—Cu1—N2A—C11A	152.2 (3)	Cu2—N2B—C11B—C10B	-44.4 (3)
O22—Cu1—N2A—C11A	-122.4 (3)	N1B—C10B—C11B—N2B	45.4 (4)
O13A—Cu1—N2A—C11A	73.4 (3)	C11B—N2B—C12B—C13B	162.2 (3)
O1B—Cu2—N1B—C7B	-11.2 (3)	Cu2—N2B—C12B—C13B	40.0 (4)
N2B—Cu2—N1B—C7B	173.6 (3)	Cu2—O2B—C13B—C12B	23.9 (4)
O2B—Cu2—N1B—C7B	-169.0 (4)	N2B—C12B—C13B—O2B	-41.6 (4)
O1M—Cu2—N1B—C7B	85.1 (3)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2A—H2A $\cdots$ O1B	0.76 (3)	1.93 (3)	2.664 (3)	162 (3)
O2B—H2B $\cdots$ O1A	0.90 (3)	1.80 (3)	2.673 (3)	164 (3)
N2A—H2AA $\cdots$ O13C <sup>i</sup>	0.91	2.52	3.134 (8)	126
N2A—H2AA $\cdots$ O12A <sup>i</sup>	0.91	2.54	3.303 (7)	142
N2B—H2BA $\cdots$ O21 <sup>ii</sup>	0.91	2.31	3.130 (4)	149
O1M—H1M $\cdots$ O14C <sup>iii</sup>	0.82	2.06	2.791 (9)	149
O1M—H1M $\cdots$ O11B <sup>iii</sup>	0.82	2.17	2.976 (10)	168
O1M—H1M $\cdots$ O14A <sup>iii</sup>	0.82	2.20	2.968 (7)	155
O1M—H1M $\cdots$ O13D <sup>iii</sup>	0.82	2.41	3.095 (11)	141
O1M—H1M $\cdots$ O12D <sup>iii</sup>	0.82	2.49	3.159 (11)	139
O1M—H1M $\cdots$ O13A <sup>iii</sup>	0.82	2.65	3.266 (7)	133

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

Fig. 1

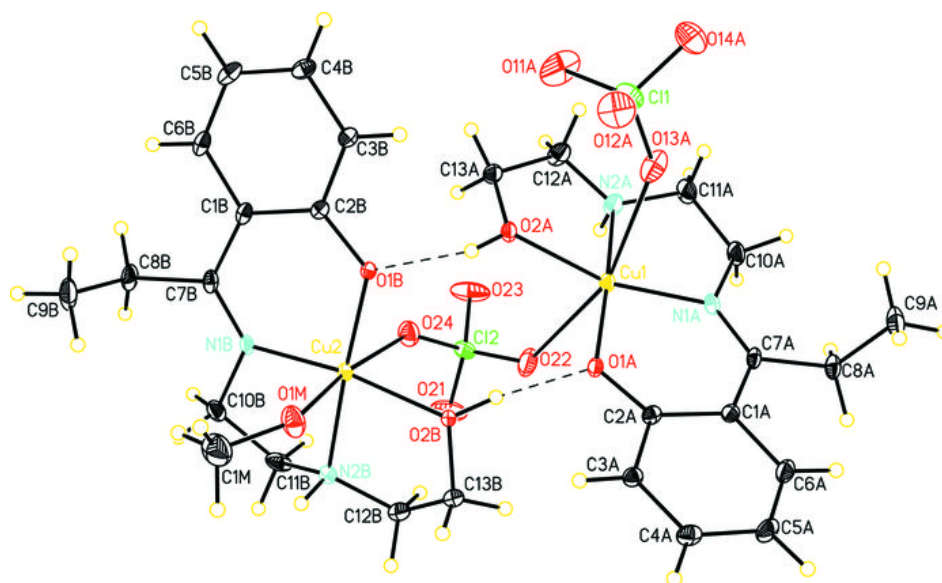




Fig. 2

