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## Structure Reports

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# Poly[[aquabis[ $\mu_2$ -6-(pyridine-3-carboxamido)naphthalene-2-carboxylato]-copper(II)] dihydrate]

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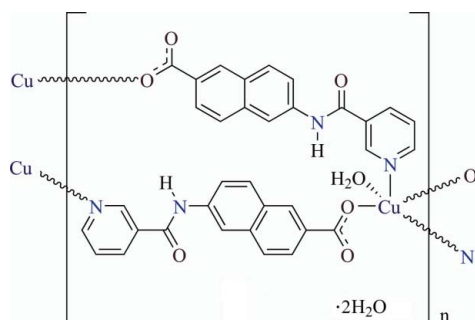
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.095; data-to-parameter ratio = 15.8.

The title compound,  $\{[\text{Cu}(\text{C}_{17}\text{H}_{11}\text{N}_2\text{O}_3)_2(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}\}_n$ , is a two-dimensional polymer. The  $\text{Cu}^{2+}$  ion lies on the crystallographic twofold axis. The coordination sphere of the  $\text{Cu}^{2+}$  ion can be described as a distorted square pyramid. All of the H atoms in the amide group and lattice water molecules participate in  $\text{O}-\text{H} \cdots \text{O}$  or  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonding to strengthen the two-dimensional framework of the polymer.

## Related literature

For coordination polymers based on linking ligands with O- and N-donor atoms, see: Robin & Fromm (2006). For  $d-f$  coordination polymers based on linking ligands with pyridyl-carboxylate terminal ligands, see: Hu *et al.* (2012); Chen *et al.* (2010); Tang *et al.* (2010); Yue *et al.* (2011); Zhu *et al.* (2010). For related potential linking ligands, see: Han & Lee (2012); Zheng & Lee (2012). For the ligand used for the preparation of the title compound, see: Song & Lee (2012).



## Experimental

### Crystal data

$[\text{Cu}(\text{C}_{17}\text{H}_{11}\text{N}_2\text{O}_3)_2(\text{H}_2\text{O})] \cdot 2\text{H}_2\text{O}$   
 $M_r = 700.14$

Monoclinic,  $C2/c$   
 $a = 29.6255$  (8) Å

$b = 6.8582$  (2) Å  
 $c = 14.8264$  (4) Å  
 $\beta = 94.728$  (3)°  
 $V = 3002.14$  (14) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.79$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.18 \times 0.16 \times 0.16$  mm

### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.870$ ,  $T_{\max} = 0.884$

24367 measured reflections  
 3705 independent reflections  
 2462 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.071$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.095$   
 $S = 1.00$   
 3705 reflections  
 234 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.28$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N1}-\text{H1} \cdots \text{O5}^i$	0.81 (3)	2.07 (3)	2.857 (4)	164 (3)
$\text{O5}-\text{H51} \cdots \text{O2}^{ii}$	0.75 (4)	2.13 (4)	2.861 (3)	164 (4)
$\text{O5}-\text{H52} \cdots \text{O3}$	0.77 (4)	2.04 (4)	2.811 (4)	177 (5)
$\text{O4}-\text{H4} \cdots \text{O2}^{iii}$	0.90 (3)	1.95 (3)	2.820 (3)	163 (3)

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Bruker, 2008); 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: AA2070).

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## supporting information

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## Poly[[aquabis[ $\mu_2$ -6-(pyridine-3-carboxamido)naphthalene-2-carboxylato]copper(II)] dihydrate]

Yun-Sung Song and Soon W. Lee

### S1. Comment

Coordination polymers are prepared by employing a wide variety of linking ligands possessing pyridyl–pyridyl, pyridyl–amine, furan–furan, thiophene–thiophene, or pyridyl–carboxylate terminals. For instance, bis(pyridyl)- and dicarboxylate-type linking ligands have long been utilized in preparing such polymers (Robin & Fromm, 2006). In particular, those containing the pyridyl–carboxylate terminals are intriguing due to the presence of both a harder carboxylate oxygen donor and a softer pyridyl nitrogen donor in them. The ligands of this type were employed to prepare unique polymers containing both *d*- and *f*-block metals within their frameworks (Hu *et al.*, 2012; Chen *et al.*, 2010; Tang *et al.*, 2010; Yue *et al.*, 2011; Zhu *et al.*, 2010). 6-(Nicotinamido)-2-naphthoic acid (HL) belongs to the pyridyl–carboxylate-type linking ligands, and we recently reported its preparation and structure (Song & Lee, 2012). Our research group also reported the molecular structures of two other related linking ligands (Han & Lee, 2012; Zheng & Lee, 2012). We report herein the structure of a two-dimensional Cu polymer of the HL ligand, which is the first *d*-block coordination polymer of this ligand.

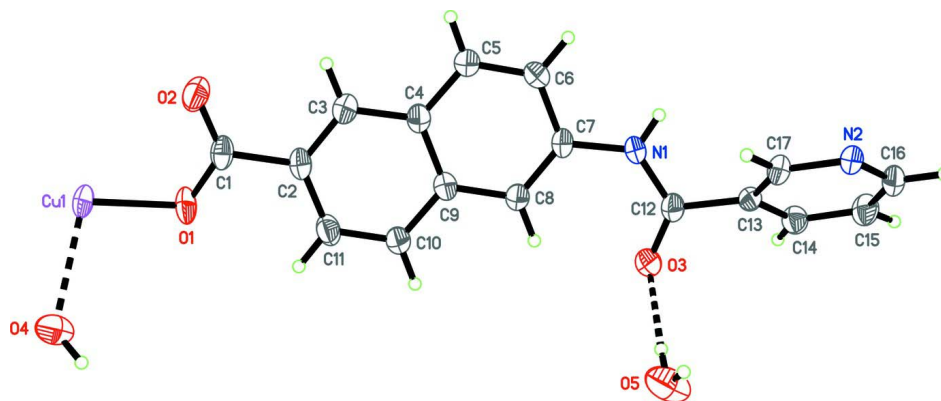
Fig. 1 shows an asymmetric unit of the title polymer, which consists of one half  $\text{Cu}^{2+}$  ion, one 6-(nicotinamido)-2-naphthoato ligand (*L*), one half aqua ligand, and one lattice water molecule. The Cu1 and O4 atoms lie on the crystallographic twofold axis, and the remaining atoms occupy general positions. The  $\text{Cu}^{2+}$  ion is coordinated to two oxygen atoms from two ligands and two nitrogen atoms from another two ligands to form a distorted square plane. The Cu1...O4 length (2.490 (3) Å), which is represented by a dotted line in Fig. 1, is extremely long, considering the covalent radii of Cu (1.28 Å) and O (0.66 Å) atoms. The van der Waals radii of Cu and O atoms are 1.40 and 1.52 Å, respectively, and therefore the Cu1...O4 bond may be best described as a strong van der Waals contact. Consequently, the coordination sphere of the  $\text{Cu}^{2+}$  ion may be thought of as square pyramidal, if the Cu1...O4 van der Waals contact is included. The molecular plane, defined by the two O and two N atoms, is extremely distorted from the planarity with the average atomic displacement of 0.328 (1) Å. Two carboxylate oxygen atoms act differently; one (O1) is coordinated to the  $\text{Cu}^{2+}$  ion and the other (O2) acts as a H-bond acceptor. The terminal carboxylate and pyridyl groups are bonded to the  $\text{Cu}^{2+}$  ions, indicating that this ligand behaves as a linking ligand. The amide group (–CONH–) does not coordinate to the metal ion, and the carbonyl oxygen (O3) acts as a H-bond acceptor and the N–H bond behaves as a H-bond donor. In fact, all of the hydrogen atoms in the amide group and lattice water molecule participate in the hydrogen bonds of the O–H...O or N–H...O types (Table 1). Fig. 2 shows a projection of the title polymer along the *c*-axis. The repeat unit consists of four ligands and four  $\text{Cu}^{2+}$  ions. This unit contains 56 atoms (4  $\text{Cu}^{2+}$  ions and 52 ligand atoms) with the  $\text{Cu}^{2+}$ ... $\text{Cu}^{2+}$  separation of 15.2045 (4) Å. The repeat units are connected by the ligands to form a 2-D layer in the [110] direction.

## S2. Experimental

A mixture of  $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$  (48.3 mg, 0.2 mmol) and 6-(nicotinamido)-2-naphthoic acid (58.4 mg, 0.2 mmol) in  $\text{H}_2\text{O}$  (20 ml) was sealed in a 24 ml Teflon-lined vessel. The reaction mixture was heated  $150\text{ }^\circ\text{C}$  for 72 h and then slowly air-cooled to room temperature for 24 h. The resulting green crystals were isolated by filtration, washed by methanol (10 ml  $\times$  3), and then air-dried to give the title compound (19 mg, 0.027 mmol, 27% yield). mp: 586–589 K. IR (KBr,  $\text{cm}^{-1}$ ): 3474 (w), 2897 (w), 2633 (w), 2383 (w), 2298 (w), 2084 (w), 1805 (w), 1660 (m), 1580 (m), 1483 (m), 1353 (m), 1204 (w), 1108 (w), 1049 (w), 951 (w), 886 (w), 824 (w), 772 (w), 749 (w), 702 (w), 625 (w), 457 (w).

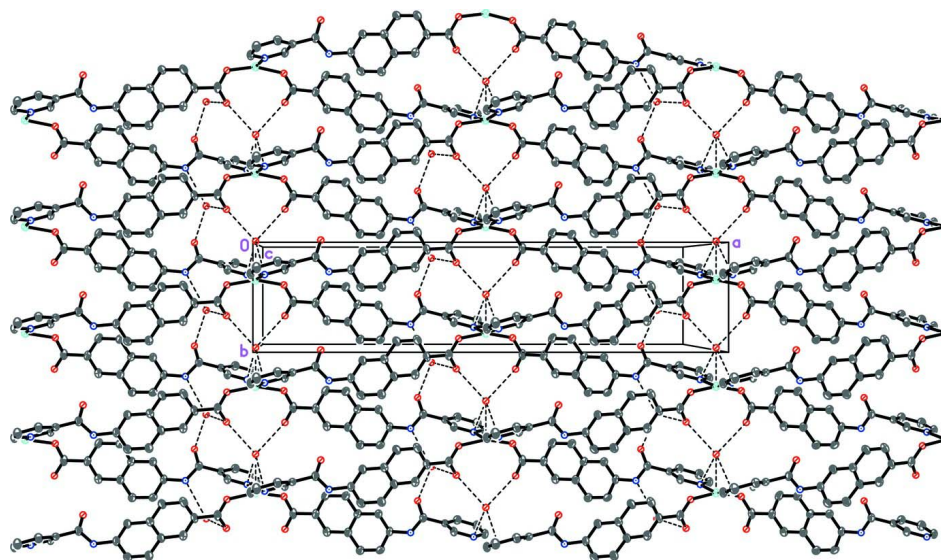
## S3. Refinement

C-bound H atoms were positioned geometrically [ $\text{C}-\text{H} = 0.93\text{ \AA}$ ] and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H-atoms participating in the H-bonds were located in a difference Fourier map and refined freely.



**Figure 1**

An asymmetric unit of the title compound showing the atomic numbering and 50% probability displacement ellipsoids.



**Figure 2**

Packing diagram of the title compound, showing a 2-D layer in the  $[110]$  direction. Dotted lines represent hydrogen bonds.

Poly[[aquabis[ $\mu_2$ -6-(pyridine-3-carboxamido)naphthalene-2-carboxylato]copper(II)] dihydrate]

## Crystal data

[Cu(C<sub>17</sub>H<sub>11</sub>N<sub>2</sub>O<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O)]·2H<sub>2</sub>O  
 $M_r = 700.14$   
 Monoclinic,  $C2/c$   
 Hall symbol:  $-C\ 2yc$   
 $a = 29.6255\ (8)\ \text{\AA}$   
 $b = 6.8582\ (2)\ \text{\AA}$   
 $c = 14.8264\ (4)\ \text{\AA}$   
 $\beta = 94.728\ (3)^\circ$   
 $V = 3002.14\ (14)\ \text{\AA}^3$   
 $Z = 4$

$F(000) = 1444$   
 $D_x = 1.549\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 3663 reflections  
 $\theta = 2.8\text{--}26.3^\circ$   
 $\mu = 0.79\ \text{mm}^{-1}$   
 $T = 296\ \text{K}$   
 Block, green  
 $0.18 \times 0.16 \times 0.16\ \text{mm}$

## Data collection

Bruker APEXII CCD  
 diffractometer  
 Radiation source: sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.870$ ,  $T_{\max} = 0.884$

24367 measured reflections  
 3705 independent reflections  
 2462 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.071$   
 $\theta_{\max} = 28.3^\circ$ ,  $\theta_{\min} = 1.4^\circ$   
 $h = -38 \rightarrow 39$   
 $k = -9 \rightarrow 8$   
 $l = -19 \rightarrow 19$

## Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.095$   
 $S = 1.00$   
 3705 reflections  
 234 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

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  
 $w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 3.3539P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.31\ \text{e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28\ \text{e \AA}^{-3}$

## Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.5000	0.15958 (7)	0.7500	0.02730 (14)
O1	0.43940 (5)	0.1123 (3)	0.69567 (11)	0.0339 (5)
O2	0.43602 (6)	-0.1766 (3)	0.76371 (12)	0.0404 (5)

O3	0.14263 (6)	0.0207 (3)	0.50325 (12)	0.0388 (5)
O4	0.5000	0.5226 (5)	0.7500	0.0458 (8)
O5	0.11363 (10)	0.3690 (4)	0.58013 (19)	0.0586 (7)
N1	0.15983 (7)	-0.2657 (4)	0.57653 (15)	0.0298 (5)
N2	0.02186 (6)	-0.2919 (3)	0.62447 (13)	0.0248 (5)
C1	0.41869 (8)	-0.0433 (4)	0.71535 (16)	0.0286 (6)
C2	0.36998 (8)	-0.0565 (4)	0.67842 (16)	0.0278 (6)
C3	0.34545 (8)	-0.2230 (4)	0.69110 (17)	0.0315 (6)
H3	0.3597	-0.3288	0.7207	0.038*
C4	0.29901 (8)	-0.2372 (4)	0.66017 (16)	0.0277 (6)
C5	0.27238 (8)	-0.4042 (4)	0.67428 (18)	0.0348 (7)
H5	0.2857	-0.5120	0.7037	0.042*
C6	0.22799 (8)	-0.4089 (4)	0.64557 (17)	0.0337 (6)
H6	0.2111	-0.5201	0.6555	0.040*
C7	0.20668 (8)	-0.2475 (4)	0.60056 (16)	0.0274 (6)
C8	0.23130 (8)	-0.0832 (4)	0.58502 (16)	0.0286 (6)
H8	0.2174	0.0225	0.5550	0.034*
C9	0.27774 (8)	-0.0746 (4)	0.61459 (16)	0.0269 (6)
C10	0.30397 (8)	0.0933 (4)	0.60178 (18)	0.0337 (7)
H10	0.2906	0.2001	0.5716	0.040*
C11	0.34869 (8)	0.1023 (4)	0.63273 (17)	0.0336 (7)
H11	0.3652	0.2148	0.6234	0.040*
C12	0.13114 (8)	-0.1337 (4)	0.53628 (16)	0.0268 (6)
C13	0.08218 (8)	-0.1870 (4)	0.53737 (16)	0.0247 (5)
C14	0.05252 (8)	-0.1765 (4)	0.45994 (16)	0.0295 (6)
H14	0.0624	-0.1341	0.4053	0.035*
C15	0.00809 (9)	-0.2305 (4)	0.46597 (17)	0.0329 (7)
H15	-0.0123	-0.2295	0.4147	0.040*
C16	-0.00604 (8)	-0.2859 (4)	0.54859 (16)	0.0292 (6)
H16	-0.0362	-0.3207	0.5518	0.035*
C17	0.06539 (8)	-0.2429 (4)	0.61731 (16)	0.0262 (6)
H17	0.0852	-0.2471	0.6692	0.031*
H1	0.1478 (10)	-0.368 (5)	0.588 (2)	0.055 (11)*
H4	0.4757 (10)	0.599 (6)	0.754 (3)	0.083 (13)*
H51	0.1036 (13)	0.338 (6)	0.623 (2)	0.072 (14)*
H52	0.1223 (14)	0.273 (7)	0.561 (3)	0.088 (17)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0144 (2)	0.0424 (3)	0.0249 (2)	0.000	0.00091 (16)	0.000
O1	0.0186 (8)	0.0527 (14)	0.0301 (9)	-0.0109 (9)	0.0001 (7)	0.0015 (9)
O2	0.0268 (9)	0.0467 (14)	0.0464 (11)	0.0048 (10)	-0.0051 (8)	0.0007 (10)
O3	0.0274 (10)	0.0329 (12)	0.0565 (12)	-0.0030 (9)	0.0062 (9)	0.0119 (10)
O4	0.052 (2)	0.032 (2)	0.0547 (19)	0.000	0.0111 (16)	0.000
O5	0.0766 (18)	0.0398 (17)	0.0638 (17)	-0.0107 (13)	0.0319 (14)	-0.0065 (13)
N1	0.0185 (11)	0.0281 (14)	0.0426 (13)	-0.0052 (11)	0.0013 (9)	0.0033 (11)
N2	0.0186 (10)	0.0288 (14)	0.0269 (10)	0.0003 (9)	0.0015 (8)	-0.0006 (9)

C1	0.0190 (12)	0.0431 (19)	0.0237 (12)	-0.0003 (13)	0.0028 (10)	-0.0078 (12)
C2	0.0188 (12)	0.0366 (17)	0.0281 (13)	-0.0046 (12)	0.0028 (10)	-0.0042 (12)
C3	0.0233 (13)	0.0352 (18)	0.0356 (14)	0.0019 (12)	0.0003 (11)	0.0004 (12)
C4	0.0219 (12)	0.0310 (16)	0.0299 (13)	-0.0020 (12)	0.0001 (10)	-0.0020 (11)
C5	0.0260 (14)	0.0308 (17)	0.0467 (16)	-0.0020 (12)	-0.0024 (12)	0.0081 (13)
C6	0.0278 (14)	0.0278 (16)	0.0450 (15)	-0.0059 (12)	-0.0003 (12)	0.0078 (13)
C7	0.0177 (12)	0.0326 (16)	0.0317 (13)	-0.0017 (12)	0.0021 (10)	-0.0005 (12)
C8	0.0220 (12)	0.0290 (16)	0.0343 (13)	-0.0011 (12)	-0.0003 (10)	0.0041 (12)
C9	0.0228 (12)	0.0299 (16)	0.0278 (12)	-0.0038 (11)	0.0012 (10)	-0.0008 (11)
C10	0.0256 (13)	0.0307 (17)	0.0437 (15)	-0.0045 (12)	-0.0031 (11)	0.0074 (12)
C11	0.0256 (13)	0.0376 (19)	0.0372 (14)	-0.0094 (12)	0.0001 (11)	0.0040 (12)
C12	0.0205 (12)	0.0313 (17)	0.0289 (12)	-0.0009 (12)	0.0040 (10)	-0.0020 (12)
C13	0.0204 (12)	0.0205 (15)	0.0332 (13)	0.0012 (11)	0.0031 (10)	-0.0024 (11)
C14	0.0276 (13)	0.0322 (17)	0.0286 (12)	-0.0012 (13)	0.0024 (10)	0.0016 (12)
C15	0.0281 (14)	0.0411 (18)	0.0281 (13)	-0.0006 (12)	-0.0061 (11)	0.0007 (12)
C16	0.0188 (12)	0.0349 (18)	0.0336 (13)	-0.0014 (11)	0.0003 (10)	-0.0013 (11)
C17	0.0187 (12)	0.0330 (16)	0.0265 (12)	0.0013 (11)	-0.0007 (10)	-0.0003 (11)

*Geometric parameters (Å, °)*

Cu1—O1	1.9337 (16)	C4—C9	1.424 (4)
Cu1—O1 <sup>i</sup>	1.9337 (16)	C5—C6	1.349 (3)
Cu1—N2 <sup>ii</sup>	2.0476 (19)	C5—H5	0.9300
Cu1—N2 <sup>iii</sup>	2.0476 (19)	C6—C7	1.414 (4)
O1—C1	1.277 (3)	C6—H6	0.9300
O2—C1	1.246 (3)	C7—C8	1.372 (4)
O3—C12	1.227 (3)	C8—C9	1.410 (3)
O4—H4	0.90 (3)	C8—H8	0.9300
O5—H51	0.75 (4)	C9—C10	1.410 (4)
O5—H52	0.77 (4)	C10—C11	1.367 (3)
N1—C12	1.347 (3)	C10—H10	0.9300
N1—C7	1.410 (3)	C11—H11	0.9300
N1—H1	0.81 (3)	C12—C13	1.497 (3)
N2—C16	1.341 (3)	C13—C17	1.377 (3)
N2—C17	1.345 (3)	C13—C14	1.389 (3)
N2—Cu1 <sup>iv</sup>	2.0476 (19)	C14—C15	1.377 (3)
C1—C2	1.503 (3)	C14—H14	0.9300
C2—C3	1.374 (4)	C15—C16	1.380 (3)
C2—C11	1.405 (4)	C15—H15	0.9300
C3—C4	1.417 (3)	C16—H16	0.9300
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.416 (4)		
O1—Cu1—O1 <sup>i</sup>	160.69 (12)	C8—C7—C6	120.0 (2)
O1—Cu1—N2 <sup>ii</sup>	93.07 (7)	N1—C7—C6	116.2 (2)
O1 <sup>i</sup> —Cu1—N2 <sup>ii</sup>	90.06 (7)	C7—C8—C9	120.1 (2)
O1—Cu1—N2 <sup>iii</sup>	90.06 (7)	C7—C8—H8	120.0
O1 <sup>i</sup> —Cu1—N2 <sup>iii</sup>	93.07 (7)	C9—C8—H8	120.0

N2 <sup>ii</sup> —Cu1—N2 <sup>iii</sup>	161.31 (12)	C8—C9—C10	121.8 (2)
C1—O1—Cu1	119.48 (17)	C8—C9—C4	119.8 (2)
H51—O5—H52	104 (4)	C10—C9—C4	118.4 (2)
C12—N1—C7	128.7 (2)	C11—C10—C9	121.4 (3)
C12—N1—H1	114 (2)	C11—C10—H10	119.3
C7—N1—H1	118 (2)	C9—C10—H10	119.3
C16—N2—C17	117.1 (2)	C10—C11—C2	120.7 (3)
C16—N2—Cu1 <sup>iv</sup>	123.25 (15)	C10—C11—H11	119.6
C17—N2—Cu1 <sup>iv</sup>	119.30 (15)	C2—C11—H11	119.6
O2—C1—O1	124.2 (2)	O3—C12—N1	124.8 (2)
O2—C1—C2	120.2 (2)	O3—C12—C13	121.1 (2)
O1—C1—C2	115.6 (2)	N1—C12—C13	114.1 (2)
C3—C2—C11	119.3 (2)	C17—C13—C14	118.5 (2)
C3—C2—C1	120.2 (2)	C17—C13—C12	119.8 (2)
C11—C2—C1	120.5 (2)	C14—C13—C12	121.7 (2)
C2—C3—C4	121.5 (3)	C15—C14—C13	118.4 (2)
C2—C3—H3	119.2	C15—C14—H14	120.8
C4—C3—H3	119.2	C13—C14—H14	120.8
C5—C4—C3	123.1 (2)	C14—C15—C16	119.5 (2)
C5—C4—C9	118.3 (2)	C14—C15—H15	120.2
C3—C4—C9	118.7 (2)	C16—C15—H15	120.2
C6—C5—C4	120.9 (3)	N2—C16—C15	122.8 (2)
C6—C5—H5	119.6	N2—C16—H16	118.6
C4—C5—H5	119.6	C15—C16—H16	118.6
C5—C6—C7	121.0 (3)	N2—C17—C13	123.6 (2)
C5—C6—H6	119.5	N2—C17—H17	118.2
C7—C6—H6	119.5	C13—C17—H17	118.2
C8—C7—N1	123.8 (2)		

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

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>
N1—H1 $\cdots$ O5 <sup>v</sup>	0.81 (3)	2.07 (3)	2.857 (4)	164 (3)
O5—H51 $\cdots$ O2 <sup>ii</sup>	0.75 (4)	2.13 (4)	2.861 (3)	164 (4)
O5—H52 $\cdots$ O3	0.77 (4)	2.04 (4)	2.811 (4)	177 (5)
O4—H4 $\cdots$ O2 <sup>vi</sup>	0.90 (3)	1.95 (3)	2.820 (3)	163 (3)

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