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# *catena*-Poly[[[aqua(2,2′-bipyridine-$\kappa^2N,N'$)copper(II)]-$\mu$-furan-2,5-dicarboxylato-$\kappa^2O^2$:$O^5$] dihydrate]

**Ya-Feng Li,* Yue Xu, Xiao-Lin Qin, Yong-Peng Yuan and Wen-Yuan Gao**

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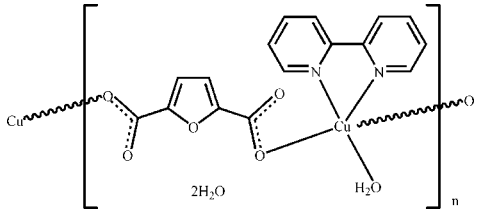
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.034; $wR$ factor = 0.092; data-to-parameter ratio = 14.5.

In the crystal structure of the title compound, $\{[Cu(C_6H_2O_5)(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O\}_n$, an infinite chain parallel to [110] is formed by the linking of $Cu(H_2O)$(2,2′-bipyridine) units through a furan-2,5-dicarboxylate bridge. The $Cu^{II}$ atom shows a square-pyramidal geometry, with one furan-2,5-dicarboxylate O atom in the apical position. The dihedral angle between the planes of the furan ring and the bipyridine molecule is 83.88 (7)°. $O_{water}$—H···O hydrogen bonds connect adjacent chains, generating a layer motif parallel to (001).

## Related literature

For a related structure, see: Li *et al.* (2012).




## Experimental

### Crystal data

$[Cu(C_6H_2O_5)(C_{10}H_8N_2)(H_2O)]\cdot 2H_2O$
$M_r$ = 427.86
Triclinic, $P\overline{1}$
$a$ = 8.8621 (18) Å
$b$ = 8.9016 (18) Å
$c$ = 12.523 (3) Å
$\alpha$ = 88.33 (3)°
$\beta$ = 69.31 (3)°
$\gamma$ = 66.85 (3)°
$V$ = 842.8 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.35 mm$^{-1}$
$T$ = 293 K
0.44 × 0.40 × 0.24 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.589, $T_{max}$ = 0.738
8312 measured reflections
3809 independent reflections
3430 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
$S$ = 1.09
3809 reflections
262 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.60 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$A$···O1$^{i}$ | 0.86 (2) | 1.87 (2) | 2.676 (2) | 156 (2) |
| O1$W$—H1$B$···O4$^{ii}$ | 0.86 (2) | 1.78 (2) | 2.623 (2) | 166 (2) |
| O2$W$—H2$A$···O5 | 0.86 (2) | 2.42 (3) | 3.211 (4) | 153 (4) |
| O2$W$—H2$B$···O2 | 0.87 (2) | 2.59 (3) | 3.353 (4) | 146 (4) |
| O3$W$—H3$A$···O4$^{iii}$ | 0.86 (2) | 2.10 (2) | 2.891 (3) | 153 (4) |
| O3$W$—H3$B$···O2 | 0.87 (2) | 1.96 (2) | 2.797 (3) | 162 (4) |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5302).

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# supporting information

*Acta Cryst.* (2012). E**68**, m1416 [doi:10.1107/S1600536812043632]

## *catena*-Poly[[[aqua(2,2′-bipyridine-$\kappa^2N,N'$)copper(II)]-$\mu$-furan-2,5-dicarboxylato-$\kappa^2O^2:O^5$] dihydrate]

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### S1. Comment

Recently, we utilized furan-2,5-dicarboxyl acid as the ligand to construct coordination polymers (Li *et al.*, 2012). As an extension of this work, a chainlike compound, $[Cu(H_2O)(C_{10}H_8N_2)(C_6H_2O_5)]\cdot 2H_2O$ (I), is now determined.

The asymmetric unit of (I) is consisted of one Cu(II) cation, one furan-2,5-dicarboxylate anion, one 2,2′-bipyridine and three water molecule The Cu atom is coordinated by two N atoms of 2,2′-bipyridine, one water O atoms and two carboxylate O atoms, exhibiting distorted square pyramid. Adjacent Cu atoms are connected by the furan-2,5-dicarboxylate to form an infinite chain (Fig. 2); $O_{water}$—H···O hydrogen bonds hold together ajacent chains to form a layer motif (Fig. 3).

### S2. Experimental

Furan-2,5-dicarboxyl acid (0.0156 g, 0.10 mmol), $Cu(NO_3)_2\cdot 6H_2O$ (0.0298 g, 0.10 mmol), 2,2′-bipyridine (0.0156, 0.10 mmol) and NaOH (0.004, 0.10 mmol) were dissolved in water (5 ml, 278 mmol) under stirring. The mixture with molar ratio of 1 (furan-2,5-dicarboxyl acid): 1 ($Cu(NO_3)_2\cdot 6H_2O$): 1 (2,2′-bipyridine): 1 NaOH: 2780 $H_2O$ was layed under room temperature for 5 days. Blue blocks were collected as a single phase.

### S3. Refinement

Water H atoms were located in a difference Fourier map and refined with O—H = 0.86 (2) Å and $U_{iso}$(H) = 1.2Ueq(O). The carbon H-atoms were placed in calculated positions (C—H (furan and pyridine ring) = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}$(H) = 1.2Ueq(C).

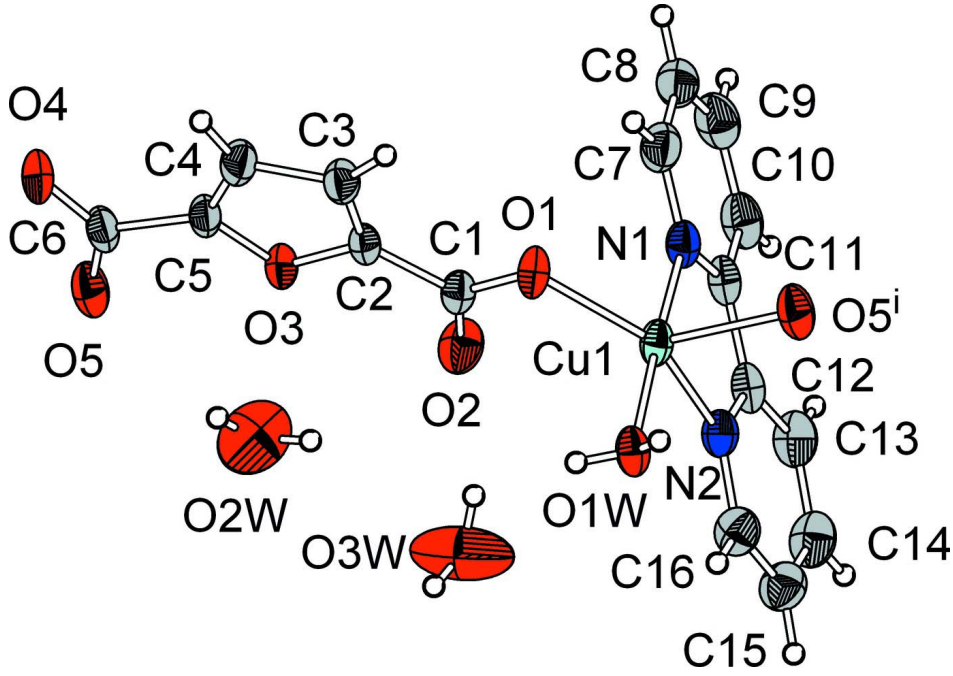


**Figure 1**

The unit cell of (I), showing the atomic labelling scheme and displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) -1 + *x*, 1 + *y*, *z*.]

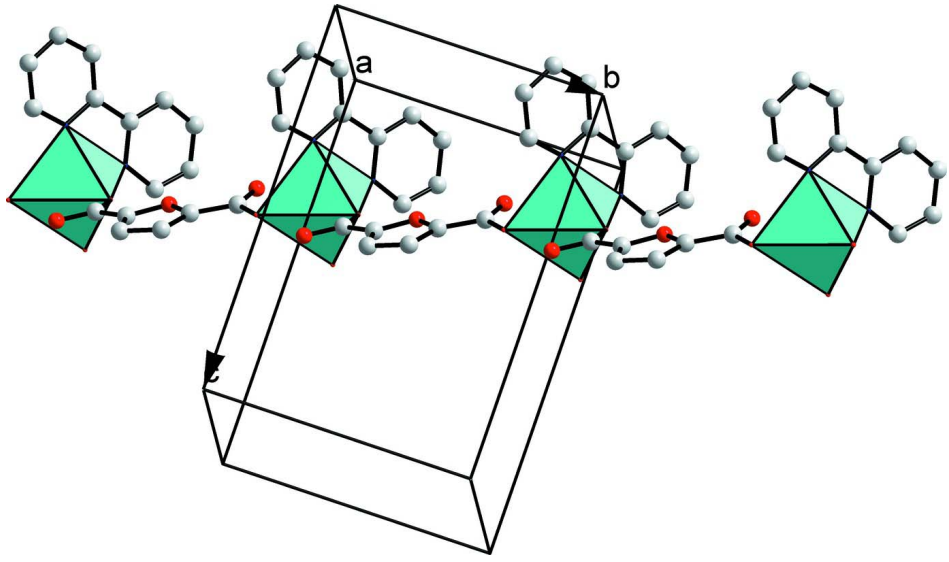


**Figure 2**

Polyhedral plot of (I), displaying the infinite chain formed by linking the adjacent Cu cations with furan-2,5-dicarboxylate.

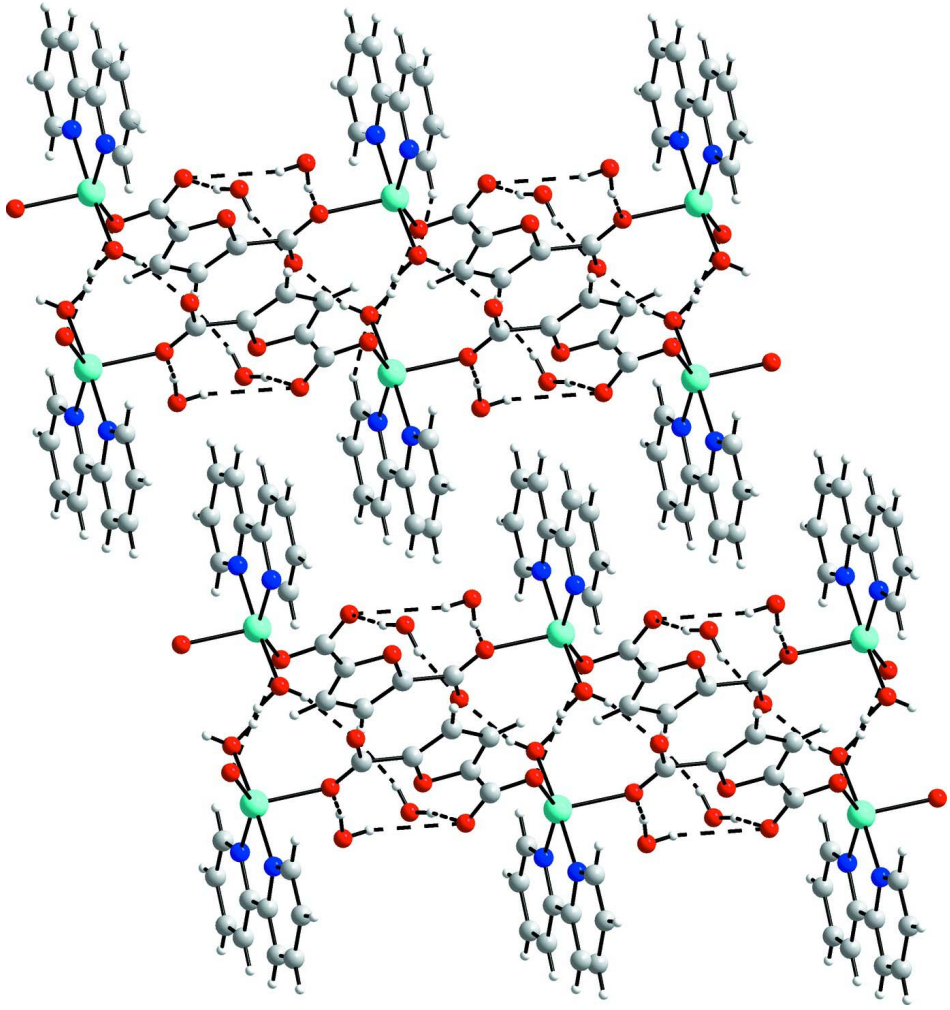

**Figure 3**

Ball-stick packing diagram of (I). The adjacent chains are holded together by the $O_{water}$–H···O H-bonding interactions to the supermolecular net.

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*Crystal data*

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$c = 12.523\ (3)$ Å
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$\beta = 69.31\ (3)°$
$\gamma = 66.85\ (3)°$
$V = 842.8\ (3)$ Å$^3$
$Z = 2$
$F(000) = 438$
$D_x = 1.686$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2000 reflections
$\theta = 3.2–27.5°$
$\mu = 1.35$ mm$^{-1}$
$T = 293$ K
Block, blue
0.44 × 0.40 × 0.24 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.00 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.589, $T_{max}$ = 0.738
8312 measured reflections
3809 independent reflections
3430 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 3.2°
$h$ = −11→11
$k$ = −10→11
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
$S$ = 1.09
3809 reflections
262 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.2206P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.60 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.11580 (3) | 1.01038 (3) | 0.296968 (19) | 0.02954 (10) |
| O1 | 0.15473 (18) | 0.80049 (16) | 0.36822 (12) | 0.0331 (3) |
| O2 | 0.4389 (2) | 0.7287 (2) | 0.26090 (15) | 0.0451 (4) |
| O3 | 0.53028 (17) | 0.43934 (16) | 0.35228 (12) | 0.0293 (3) |
| O4 | 0.6968 (2) | 0.0548 (2) | 0.45196 (17) | 0.0512 (4) |
| O5 | 0.8433 (2) | 0.19001 (19) | 0.33789 (14) | 0.0428 (4) |
| N1 | 0.1301 (2) | 0.9088 (2) | 0.15292 (15) | 0.0326 (4) |
| N2 | 0.2242 (2) | 1.1413 (2) | 0.18474 (14) | 0.0312 (3) |
| C1 | 0.3191 (3) | 0.7013 (2) | 0.33247 (16) | 0.0288 (4) |
| C2 | 0.3569 (2) | 0.5458 (2) | 0.38399 (16) | 0.0261 (4) |
| C3 | 0.2525 (3) | 0.4845 (2) | 0.46097 (19) | 0.0335 (4) |
| H3 | 0.1299 | 0.5339 | 0.4956 | 0.040* |
| C4 | 0.3660 (3) | 0.3303 (3) | 0.4786 (2) | 0.0366 (4) |
| H4 | 0.3327 | 0.2579 | 0.5265 | 0.044* |
| C5 | 0.5319 (3) | 0.3088 (2) | 0.41239 (17) | 0.0294 (4) |

| | | | | |
|---|---|---|---|---|
| C6 | 0.7064 (3) | 0.1739 (2) | 0.39860 (18) | 0.0338 (4) |
| C7 | 0.0776 (3) | 0.7887 (3) | 0.1463 (2) | 0.0421 (5) |
| H7 | 0.0250 | 0.7516 | 0.2136 | 0.050* |
| C8 | 0.0994 (4) | 0.7183 (3) | 0.0416 (2) | 0.0478 (6) |
| H8 | 0.0612 | 0.6357 | 0.0385 | 0.057* |
| C9 | 0.1790 (3) | 0.7732 (3) | −0.0579 (2) | 0.0486 (6) |
| H9 | 0.1979 | 0.7257 | −0.1292 | 0.058* |
| C10 | 0.2306 (3) | 0.8992 (3) | −0.05098 (19) | 0.0416 (5) |
| H10 | 0.2828 | 0.9386 | −0.1172 | 0.050* |
| C11 | 0.2033 (3) | 0.9656 (2) | 0.05623 (17) | 0.0320 (4) |
| C12 | 0.2515 (3) | 1.1018 (2) | 0.07481 (17) | 0.0310 (4) |
| C13 | 0.3209 (3) | 1.1829 (3) | −0.01247 (19) | 0.0409 (5) |
| H13 | 0.3389 | 1.1543 | −0.0882 | 0.049* |
| C14 | 0.3626 (3) | 1.3065 (3) | 0.0148 (2) | 0.0455 (5) |
| H14 | 0.4086 | 1.3629 | −0.0424 | 0.055* |
| C15 | 0.3359 (3) | 1.3460 (3) | 0.1276 (2) | 0.0439 (5) |
| H15 | 0.3648 | 1.4284 | 0.1472 | 0.053* |
| C16 | 0.2659 (3) | 1.2617 (3) | 0.2105 (2) | 0.0398 (5) |
| H16 | 0.2468 | 1.2889 | 0.2867 | 0.048* |
| O1W | 0.1177 (2) | 1.12059 (17) | 0.43017 (12) | 0.0325 (3) |
| H1A | 0.014 (2) | 1.164 (3) | 0.4834 (19) | 0.039* |
| H1B | 0.191 (3) | 1.056 (3) | 0.458 (2) | 0.039* |
| O2W | 0.8652 (4) | 0.5101 (4) | 0.2205 (3) | 0.0910 (9) |
| H2A | 0.832 (6) | 0.451 (5) | 0.272 (3) | 0.109* |
| H2B | 0.767 (4) | 0.599 (4) | 0.241 (4) | 0.109* |
| O3W | 0.6105 (5) | 0.9237 (5) | 0.2840 (2) | 0.1073 (12) |
| H3A | 0.611 (7) | 0.952 (6) | 0.349 (3) | 0.129* |
| H3B | 0.540 (6) | 0.876 (6) | 0.291 (4) | 0.129* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.03370 (15) | 0.02750 (14) | 0.02279 (14) | −0.00666 (10) | −0.01233 (10) | 0.00782 (9) |
| O1 | 0.0304 (7) | 0.0281 (6) | 0.0285 (7) | −0.0017 (5) | −0.0093 (6) | 0.0085 (5) |
| O2 | 0.0393 (9) | 0.0437 (9) | 0.0430 (9) | −0.0158 (7) | −0.0071 (7) | 0.0168 (7) |
| O3 | 0.0238 (6) | 0.0268 (6) | 0.0306 (7) | −0.0038 (5) | −0.0104 (5) | 0.0055 (5) |
| O4 | 0.0553 (11) | 0.0374 (8) | 0.0717 (12) | −0.0114 (7) | −0.0454 (10) | 0.0227 (8) |
| O5 | 0.0294 (8) | 0.0399 (8) | 0.0448 (9) | 0.0019 (6) | −0.0154 (7) | 0.0012 (6) |
| N1 | 0.0358 (9) | 0.0294 (8) | 0.0298 (9) | −0.0069 (7) | −0.0167 (7) | 0.0074 (6) |
| N2 | 0.0314 (8) | 0.0318 (8) | 0.0245 (8) | −0.0078 (7) | −0.0098 (7) | 0.0066 (6) |
| C1 | 0.0322 (10) | 0.0252 (8) | 0.0258 (9) | −0.0070 (7) | −0.0127 (8) | 0.0042 (7) |
| C2 | 0.0230 (8) | 0.0244 (8) | 0.0271 (9) | −0.0037 (6) | −0.0116 (7) | 0.0025 (7) |
| C3 | 0.0257 (9) | 0.0316 (9) | 0.0396 (11) | −0.0084 (7) | −0.0121 (8) | 0.0099 (8) |
| C4 | 0.0370 (11) | 0.0322 (10) | 0.0431 (12) | −0.0133 (8) | −0.0192 (9) | 0.0160 (8) |
| C5 | 0.0314 (10) | 0.0254 (8) | 0.0318 (10) | −0.0063 (7) | −0.0184 (8) | 0.0058 (7) |
| C6 | 0.0356 (11) | 0.0290 (9) | 0.0349 (11) | −0.0025 (8) | −0.0228 (9) | −0.0001 (7) |
| C7 | 0.0499 (13) | 0.0355 (11) | 0.0435 (13) | −0.0141 (9) | −0.0246 (11) | 0.0110 (9) |
| C8 | 0.0538 (14) | 0.0353 (11) | 0.0593 (16) | −0.0112 (10) | −0.0343 (13) | 0.0032 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0499 (14) | 0.0471 (13) | 0.0412 (13) | −0.0049 (10) | −0.0247 (11) | −0.0062 (10) |
| C10 | 0.0378 (11) | 0.0467 (12) | 0.0291 (11) | −0.0050 (9) | −0.0134 (9) | 0.0008 (9) |
| C11 | 0.0265 (9) | 0.0326 (9) | 0.0278 (10) | −0.0014 (7) | −0.0123 (8) | 0.0040 (7) |
| C12 | 0.0255 (9) | 0.0337 (9) | 0.0246 (9) | −0.0028 (7) | −0.0096 (8) | 0.0056 (7) |
| C13 | 0.0409 (12) | 0.0465 (12) | 0.0253 (10) | −0.0117 (9) | −0.0086 (9) | 0.0099 (8) |
| C14 | 0.0428 (13) | 0.0471 (12) | 0.0382 (12) | −0.0167 (10) | −0.0082 (10) | 0.0157 (10) |
| C15 | 0.0453 (13) | 0.0410 (12) | 0.0443 (13) | −0.0194 (10) | −0.0141 (11) | 0.0111 (9) |
| C16 | 0.0459 (12) | 0.0402 (11) | 0.0329 (11) | −0.0168 (9) | −0.0154 (10) | 0.0074 (8) |
| O1W | 0.0319 (7) | 0.0338 (7) | 0.0247 (7) | −0.0049 (6) | −0.0125 (6) | 0.0064 (5) |
| O2W | 0.0754 (18) | 0.0805 (18) | 0.091 (2) | −0.0308 (14) | −0.0024 (16) | 0.0061 (15) |
| O3W | 0.166 (3) | 0.179 (3) | 0.0414 (12) | −0.140 (3) | −0.0327 (16) | 0.0241 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1W | 1.9681 (15) | C7—H7 | 0.9300 |
| Cu1—N1 | 1.9825 (18) | C8—C9 | 1.380 (4) |
| Cu1—O1 | 2.0048 (15) | C8—H8 | 0.9300 |
| Cu1—N2 | 2.0218 (18) | C9—C10 | 1.382 (4) |
| Cu1—O5$^{i}$ | 2.1885 (18) | C9—H9 | 0.9300 |
| O1—C1 | 1.286 (2) | C10—C11 | 1.384 (3) |
| O2—C1 | 1.228 (3) | C10—H10 | 0.9300 |
| O3—C5 | 1.364 (2) | C11—C12 | 1.483 (3) |
| O3—C2 | 1.364 (2) | C12—C13 | 1.386 (3) |
| O4—C6 | 1.252 (3) | C13—C14 | 1.377 (4) |
| O5—C6 | 1.244 (3) | C13—H13 | 0.9300 |
| N1—C7 | 1.338 (3) | C14—C15 | 1.378 (4) |
| N1—C11 | 1.345 (3) | C14—H14 | 0.9300 |
| N2—C12 | 1.343 (3) | C15—C16 | 1.376 (3) |
| N2—C16 | 1.343 (3) | C15—H15 | 0.9300 |
| C1—C2 | 1.477 (2) | C16—H16 | 0.9300 |
| C2—C3 | 1.349 (3) | O1W—H1A | 0.861 (15) |
| C3—C4 | 1.413 (3) | O1W—H1B | 0.856 (16) |
| C3—H3 | 0.9300 | O2W—H2A | 0.862 (19) |
| C4—C5 | 1.346 (3) | O2W—H2B | 0.872 (19) |
| C4—H4 | 0.9300 | O3W—H3A | 0.862 (18) |
| C5—C6 | 1.493 (3) | O3W—H3B | 0.868 (18) |
| C7—C8 | 1.386 (3) | | |

| | | | |
|---|---|---|---|
| O1W—Cu1—N1 | 174.26 (7) | O5—C6—C5 | 118.49 (19) |
| O1W—Cu1—O1 | 91.08 (6) | O5—C6—C5 | 118.49 (19) |
| N1—Cu1—O1 | 92.85 (7) | O4—C6—C5 | 114.5 (2) |
| O1W—Cu1—N2 | 93.35 (7) | N1—C7—C8 | 121.7 (2) |
| N1—Cu1—N2 | 81.09 (7) | N1—C7—H7 | 119.1 |
| O1—Cu1—N2 | 147.26 (7) | C8—C7—H7 | 119.1 |
| O1W—Cu1—O5$^{i}$ | 88.22 (7) | C9—C8—C7 | 118.8 (2) |
| N1—Cu1—O5$^{i}$ | 93.61 (8) | C9—C8—H8 | 120.6 |
| O1—Cu1—O5$^{i}$ | 117.97 (7) | C7—C8—H8 | 120.6 |
| N2—Cu1—O5$^{i}$ | 94.59 (7) | C8—C9—C10 | 119.6 (2) |

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| C1—O1—Cu1 | 112.08 (13) | C8—C9—H9 | 120.2 |
| C5—O3—C2 | 106.11 (15) | C10—C9—H9 | 120.2 |
| C6—O5—Cu1$^{ii}$ | 126.72 (14) | C9—C10—C11 | 118.9 (2) |
| C7—N1—C11 | 119.63 (18) | C9—C10—H10 | 120.6 |
| C7—N1—Cu1 | 124.99 (15) | C11—C10—H10 | 120.6 |
| C11—N1—Cu1 | 115.35 (14) | N1—C11—C10 | 121.4 (2) |
| C12—N2—C16 | 119.17 (18) | N1—C11—C12 | 114.70 (17) |
| C12—N2—Cu1 | 114.27 (14) | C10—C11—C12 | 123.9 (2) |
| C16—N2—Cu1 | 126.55 (14) | N2—C12—C13 | 121.52 (19) |
| O2—C1—O1 | 124.51 (18) | N2—C12—C11 | 114.49 (18) |
| O2—C1—O1 | 124.51 (18) | C13—C12—C11 | 124.00 (18) |
| O2—C1—C2 | 120.80 (18) | C14—C13—C12 | 118.9 (2) |
| O2—C1—C2 | 120.80 (18) | C14—C13—H13 | 120.6 |
| O1—C1—C2 | 114.69 (17) | C12—C13—H13 | 120.6 |
| C3—C2—O3 | 110.33 (16) | C13—C14—C15 | 119.6 (2) |
| C3—C2—C1 | 132.79 (17) | C13—C14—H14 | 120.2 |
| O3—C2—C1 | 116.87 (17) | C15—C14—H14 | 120.2 |
| C2—C3—C4 | 106.52 (18) | C16—C15—C14 | 118.9 (2) |
| C2—C3—H3 | 126.7 | C16—C15—H15 | 120.6 |
| C4—C3—H3 | 126.7 | C14—C15—H15 | 120.6 |
| C5—C4—C3 | 106.56 (19) | N2—C16—C15 | 122.0 (2) |
| C5—C4—H4 | 126.7 | N2—C16—H16 | 119.0 |
| C3—C4—H4 | 126.7 | C15—C16—H16 | 119.0 |
| C4—C5—O3 | 110.48 (17) | Cu1—O1W—H1A | 111.7 (16) |
| C4—C5—C6 | 131.21 (19) | Cu1—O1W—H1B | 112.7 (16) |
| O3—C5—C6 | 118.28 (18) | H1A—O1W—H1B | 109.8 (19) |
| O5—C6—O4 | 127.0 (2) | H2A—O2W—H2B | 100 (4) |
| O5—C6—O4 | 127.0 (2) | H3A—O3W—H3B | 113 (3) |

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|---|---|---|---|
| O1W—Cu1—O1—C1 | −95.25 (14) | Cu1$^{ii}$—O5—C6—O5 | 0 (100) |
| N1—Cu1—O1—C1 | 80.57 (14) | O5—O5—C6—O4 | 0.00 (8) |
| N2—Cu1—O1—C1 | 2.6 (2) | Cu1$^{ii}$—O5—C6—O4 | 2.9 (3) |
| O5$^{i}$—Cu1—O1—C1 | 176.19 (12) | O5—O5—C6—C5 | 0.00 (6) |
| O1—Cu1—N1—C7 | 32.30 (18) | Cu1$^{ii}$—O5—C6—C5 | −177.61 (12) |
| N2—Cu1—N1—C7 | 179.94 (18) | C4—C5—C6—O5 | −174.2 (2) |
| O5$^{i}$—Cu1—N1—C7 | −85.97 (18) | O3—C5—C6—O5 | 3.8 (3) |
| O1—Cu1—N1—C11 | −145.90 (14) | C4—C5—C6—O5 | −174.2 (2) |
| N2—Cu1—N1—C11 | 1.74 (14) | O3—C5—C6—O5 | 3.8 (3) |
| O5$^{i}$—Cu1—N1—C11 | 95.83 (15) | C4—C5—C6—O4 | 5.4 (3) |
| O1W—Cu1—N2—C12 | 178.94 (14) | O3—C5—C6—O4 | −176.59 (17) |
| N1—Cu1—N2—C12 | 0.37 (14) | C11—N1—C7—C8 | 1.2 (3) |
| O1—Cu1—N2—C12 | 81.71 (18) | Cu1—N1—C7—C8 | −176.89 (17) |
| O5$^{i}$—Cu1—N2—C12 | −92.58 (14) | N1—C7—C8—C9 | 0.6 (4) |
| O1W—Cu1—N2—C16 | −2.47 (18) | C7—C8—C9—C10 | −1.7 (4) |
| N1—Cu1—N2—C16 | 178.95 (19) | C8—C9—C10—C11 | 1.0 (3) |
| O1—Cu1—N2—C16 | −99.7 (2) | C7—N1—C11—C10 | −2.0 (3) |
| O5$^{i}$—Cu1—N2—C16 | 86.00 (18) | Cu1—N1—C11—C10 | 176.33 (15) |
| O2—O2—C1—O1 | 0.00 (8) | C7—N1—C11—C12 | 178.33 (18) |

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| O2—O2—C1—C2 | 0.00 (14) | Cu1—N1—C11—C12 | −3.4 (2) |
| Cu1—O1—C1—O2 | −1.8 (3) | C9—C10—C11—N1 | 0.9 (3) |
| Cu1—O1—C1—O2 | −1.8 (3) | C9—C10—C11—C12 | −179.47 (19) |
| Cu1—O1—C1—C2 | 178.61 (12) | C16—N2—C12—C13 | −0.3 (3) |
| C5—O3—C2—C3 | −0.3 (2) | Cu1—N2—C12—C13 | 178.40 (16) |
| C5—O3—C2—C1 | 178.50 (15) | C16—N2—C12—C11 | 179.10 (17) |
| O2—C1—C2—C3 | −178.6 (2) | Cu1—N2—C12—C11 | −2.2 (2) |
| O2—C1—C2—C3 | −178.6 (2) | N1—C11—C12—N2 | 3.7 (2) |
| O1—C1—C2—C3 | 1.1 (3) | C10—C11—C12—N2 | −176.01 (19) |
| O2—C1—C2—O3 | 2.9 (3) | N1—C11—C12—C13 | −176.94 (19) |
| O2—C1—C2—O3 | 2.9 (3) | C10—C11—C12—C13 | 3.4 (3) |
| O1—C1—C2—O3 | −177.42 (16) | N2—C12—C13—C14 | 0.1 (3) |
| O3—C2—C3—C4 | −0.2 (2) | C11—C12—C13—C14 | −179.3 (2) |
| C1—C2—C3—C4 | −178.8 (2) | C12—C13—C14—C15 | 0.5 (3) |
| C2—C3—C4—C5 | 0.7 (2) | C13—C14—C15—C16 | −0.8 (4) |
| C3—C4—C5—O3 | −0.9 (2) | C12—N2—C16—C15 | 0.0 (3) |
| C3—C4—C5—C6 | 177.18 (19) | Cu1—N2—C16—C15 | −178.54 (18) |
| C2—O3—C5—C4 | 0.8 (2) | C14—C15—C16—N2 | 0.5 (4) |
| C2—O3—C5—C6 | −177.60 (15) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O1$^{iii}$ | 0.86 (2) | 1.87 (2) | 2.676 (2) | 156 (2) |
| O1*W*—H1*B*···O4$^{iv}$ | 0.86 (2) | 1.78 (2) | 2.623 (2) | 166 (2) |
| O2*W*—H2*A*···O5 | 0.86 (2) | 2.42 (3) | 3.211 (4) | 153 (4) |
| O2*W*—H2*B*···O2 | 0.87 (2) | 2.59 (3) | 3.353 (4) | 146 (4) |
| O3*W*—H3*A*···O4$^{v}$ | 0.86 (2) | 2.10 (2) | 2.891 (3) | 153 (4) |
| O3*W*—H3*B*···O2 | 0.87 (2) | 1.96 (2) | 2.797 (3) | 162 (4) |

Symmetry codes: (iii) $-x, -y+2, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $x, y+1, z$.