# Di-$\mu$-glutarato-$\kappa^4O^1$:$O^5$-bis[aqua(1,10-phenanthroline-$\kappa^2N$,$N'$)copper(II)]

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In the centrosymmetric dinuclear title complex, [Cu$_2$-(C$_5$H$_6$O$_4$)$_2$(C$_{12}$H$_{18}$N$_2$)$_2$(H$_2$O)$_2$], the Cu$^{II}$ atom displays a distorted square-pyramidal coordination environment with the basal plane occupied by two phenanthroline N atoms and two O atoms from different glutarate dianions while a water molecule is located at the apical position. Of the two water H atoms, one is engaged in an intramolecular hydrogen bond with a free oxygen of the dianion whereas the second is engaged in an intermolecular hydrogen bond, building a corrugated layer parallel to (100). These layers are further connected through $\pi$–$\pi$ stacking interactions involving symmetry-related phenanthroline rings [centroid–centroid distance = 3.5599 (17) and 3.5617 (18) Å], building a three dimensionnal network. C—H$\cdots\pi$ interactions involving the phenanthroline ring system are also observed.

## Related literature

For coordination modes of the glutarate anion, see: Ghosh *et al.* (2007); Kim *et al.* (2005); Rather & Zaworotko (2003); Zheng *et al.* (2004); Vaidhyanathan *et al.* (2004); Girginova *et al.* (2007).
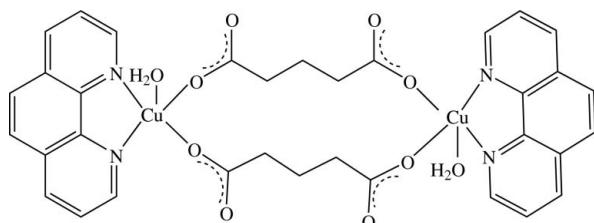


## Experimental

### Crystal data

[Cu$_2$(C$_5$H$_6$O$_4$)$_2$(C$_{12}$H$_{18}$N$_2$)$_2$(H$_2$O)$_2$]
$M_r$ = 783.72
Monoclinic, $P2_1/c$
$a$ = 10.2767 (11) Å
$b$ = 10.5935 (14) Å
$c$ = 15.5998 (16) Å
$\beta$ = 107.114 (1)°
$V$ = 1623.1 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.38 mm$^{-1}$
$T$ = 298 K
0.26 × 0.25 × 0.23 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.716, $T_{max}$ = 0.742
7937 measured reflections
2867 independent reflections
2275 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
$S$ = 1.07
2867 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

$Cg1$ is the centroid of the N1,C6–C10 ring

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O5—H51$\cdots$O4 | 0.89 | 1.81 | 2.659 (3) | 158 |
| O5—H52$\cdots$O2$^i$ | 0.88 | 1.89 | 2.762 (3) | 169 |
| C2—H2A$\cdots$Cg1$^i$ | 0.97 | 2.88 | 3.754 (3) | 151 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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# supporting information

# Di-*μ*-glutarato-*κ*⁴*O*¹:*O*⁵-bis[aqua(1,10-phenanthroline-*κ*²*N*,*N*′)copper(II)]

## Yong-Hong Zhou

### S1. Comment

For many yeras, there is a growing interest in developing organic-inorganic hybrid materials owing to their intriguing structures, new topologies, and potential applications(Ghosh *et al.*, 2007; Kim *et al.*,2005). Carboxylic acids have been proved to be versatile functional moieties in generating interesting hybrid materials by interacting with metal ions. The abilities of its anion to metal ions in diverse and unique linking modes can be regarded as a major factor in making the carboxylate function a versatile structure directing moiety.

Metal glutarates are one class of dicarboxylate system which exhibit interesting structural features. Previous investigations have demonstrated that glutaric acid presents interesting behaviors due to its conformational flexibility and coordination diversity (Rather *et al.*, 2003; Zheng *et al.*, 2004; Vaidhyanathan *et al.*, 2004; Girginova *et al.*, 2007). We report here the crystal structure of the title compound.

The title complex, $[Cu(C_{12}H_{18}N_2)(C_5H_6O_4)(H_2O)]_2$, is a dinuclear compound organized around inversion center. The $Cu^{II}$ displays a distorted square pyramidal coordination environment (Fig. 1). The basal plane is occupied by two nitrogen atoms of the phenanthroline [Cu—N(1) = 2.014 (2)Å and Cu—N(2) = 2.022 (2) Å] and two O atoms from different glutarate dianions[Cu—O(1) = 1.954 (2)Å and Cu—O(3) = 1.947 (2) Å], whereas one water molecule is located at the apical position at a significantly longer distance[Cu—O(5) = 2.380 (2) Å]. The glutarate dianions act as a bidentate ligand bridging the two $Cu^{II}$ ions which are separated by 8.476 Å.

There is an intramolecular hydrogen bond involving one H of the water and the O4 oxygen of one dianion within the dinuclear complex. The second H atom of the water is engaged in hydrogen bond interaction with the O2 oxygen atom of symmetry related dinuclear complex building then a corrugated layer parallel to the (1 0 0) plane (Fig. 2, Table 1). The layers are interconnected through $\pi$-$\pi$ stacking involving the symmetry related N1,C6,C7,C8,C9,C10 (A) and N2,C11,C12,C13,C14,C15 (B) phenanthroline rings (Fig. 2, Table 2) building a three dimensional network. The packing is further stabilized by weak C—H⋯$\pi$ interaction involving the symmetry related ring A (Table 1).

### S2. Experimental

The title complex was prepared by the addition of the stoichiometric amount of $CuCl_2$ (0.134 g, 1 mmol) to an ethanol solution of glutaric acid (0.264 g, 2 mmol) and 1,10-phenanthroline monohydrate(0.396 g, 2 mmol), the pH was adjusted to ~6 with 0.2 mol.$L^{-1}$ KOH solution. The resulting solution was stirred for 30 min at room temperature and then filtered. Blue single crystals were isolated from the solution at room temperature over two weeks.

### S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene) with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H= 0.88 (1)Å and H⋯H= 1.50 (2) Å) with $U_{iso}(H) = 1.5U_{eq}(O)$. In the last

cycles of refinement, they were treated as riding on their parent O atoms.
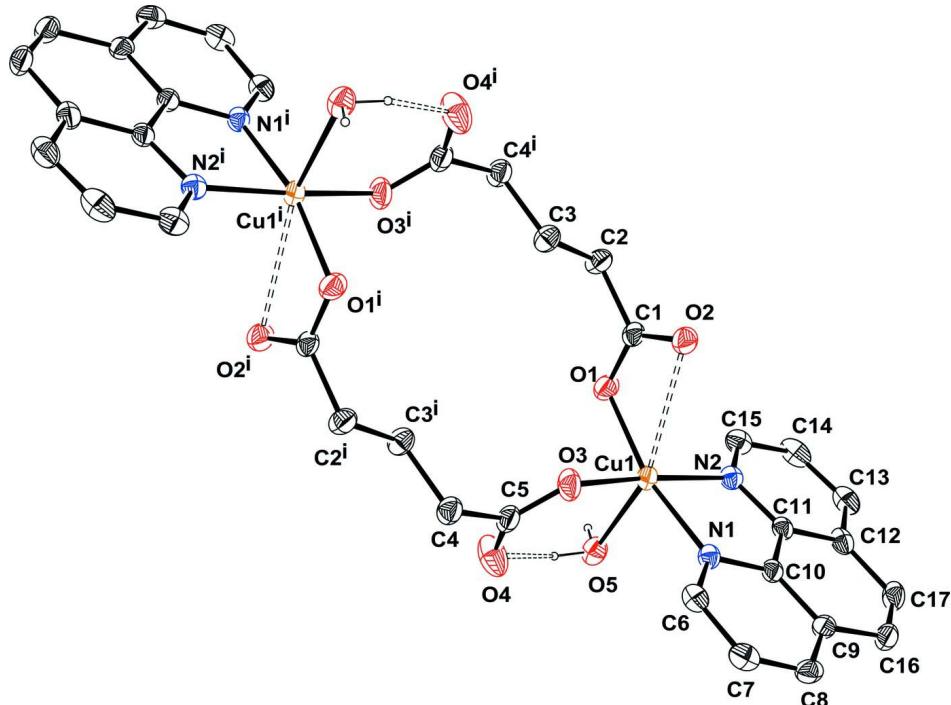


## Figure 1

The molecular structure of the title compound with the atom labeling scheme. Displacement thermal paremeters are represented at the 30% probability level. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for the sake of clarity. [Symmetry code: (i) -$x$ + 1, -$y$ + 1, -$z$ + 1]
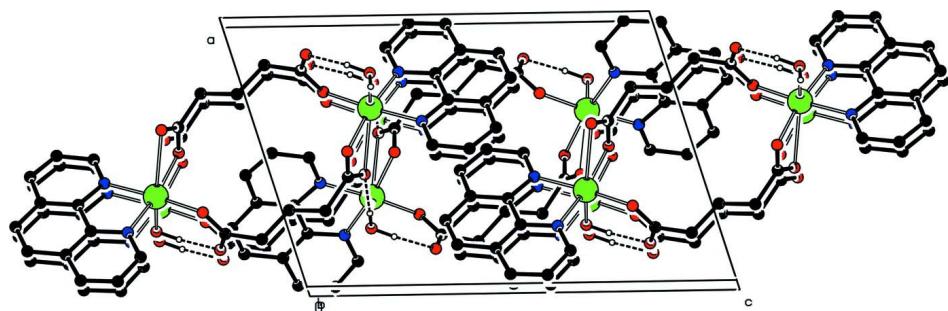


## Figure 2

Partial packing view showing the formation of layer through O—H···O hydrogen bonds which are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for the sake of clarity.

**Di-μ-glutarato-κ⁴$O^1$:$O^5$-bis[aqua(1,10-phenanthroline-κ²$N$,$N′$)copper(II)]**

*Crystal data*
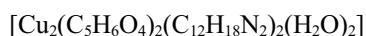
| | |
|---|---|
| $[Cu_2(C_5H_6O_4)_2(C_{12}H_{18}N_2)_2(H_2O)_2]$ | $c$ = 15.5998 (16) Å |
| $M_r$ = 783.72 | $\beta$ = 107.114 (1)° |
| Monoclinic, $P2_1/c$ | $V$ = 1623.1 (3) Å$^3$ |
| Hall symbol: -P 2ybc | $Z$ = 2 |
| $a$ = 10.2767 (11) Å | $F(000)$ = 804 |
| $b$ = 10.5935 (14) Å | $D_x$ = 1.604 Mg m$^{-3}$ |

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3334 reflections
$\theta = 2.4–27.3°$
$\mu = 1.38$ mm$^{-1}$

$T = 298$ K
Block, blue
$0.26 \times 0.25 \times 0.23$ mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.716$, $T_{max} = 0.742$

7937 measured reflections
2867 independent reflections
2275 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 12$
$k = -12 \rightarrow 10$
$l = -18 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.083$
$S = 1.07$
2867 reflections
226 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 1.103P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.28$ 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 (Å$^2$)*

|  | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.34382 (3) | 0.54797 (3) | 0.21857 (2) | 0.03292 (13) |
| N1 | 0.2087 (2) | 0.4429 (2) | 0.12652 (14) | 0.0299 (5) |
| N2 | 0.3977 (2) | 0.6012 (2) | 0.10928 (14) | 0.0318 (5) |
| O1 | 0.5068 (2) | 0.61750 (19) | 0.30440 (12) | 0.0416 (5) |
| O2 | 0.5850 (2) | 0.43066 (19) | 0.28151 (13) | 0.0432 (5) |
| O3 | 0.2798 (2) | 0.4813 (2) | 0.31524 (13) | 0.0467 (5) |
| O4 | 0.1462 (3) | 0.6404 (2) | 0.32731 (17) | 0.0689 (7) |
| O5 | 0.2215 (2) | 0.74242 (19) | 0.19357 (13) | 0.0441 (5) |
| H51 | 0.1900 | 0.7287 | 0.2401 | 0.066* |
| H52 | 0.2746 | 0.8093 | 0.2014 | 0.066* |
| C1 | 0.5979 (3) | 0.5330 (3) | 0.32214 (17) | 0.0318 (6) |
| C2 | 0.7228 (3) | 0.5601 (3) | 0.39982 (18) | 0.0397 (7) |

| | | | |
|---|---|---|---|
| H2A | 0.7284 | 0.6499 | 0.4125 | 0.048* |
| H2B | 0.8038 | 0.5354 | 0.3841 | 0.048* |
| C3 | 0.7158 (3) | 0.4873 (3) | 0.48313 (18) | 0.0380 (7) |
| H3A | 0.6265 | 0.4993 | 0.4910 | 0.046* |
| H3B | 0.7266 | 0.3980 | 0.4735 | 0.046* |
| C4 | 0.1767 (3) | 0.4723 (3) | 0.43155 (18) | 0.0401 (7) |
| H4A | 0.1805 | 0.3816 | 0.4242 | 0.048* |
| H4B | 0.0869 | 0.4938 | 0.4356 | 0.048* |
| C5 | 0.2012 (3) | 0.5385 (3) | 0.35137 (18) | 0.0387 (7) |
| C6 | 0.1142 (3) | 0.3640 (3) | 0.13755 (19) | 0.0370 (7) |
| H6 | 0.1091 | 0.3496 | 0.1953 | 0.044* |
| C7 | 0.0230 (3) | 0.3025 (3) | 0.0664 (2) | 0.0417 (7) |
| H7 | −0.0423 | 0.2487 | 0.0768 | 0.050* |
| C8 | 0.0291 (3) | 0.3208 (3) | −0.0187 (2) | 0.0401 (7) |
| H8 | −0.0321 | 0.2800 | −0.0667 | 0.048* |
| C9 | 0.1287 (3) | 0.4017 (3) | −0.03337 (18) | 0.0339 (6) |
| C10 | 0.2164 (3) | 0.4611 (2) | 0.04186 (17) | 0.0292 (6) |
| C11 | 0.3172 (3) | 0.5485 (2) | 0.03226 (17) | 0.0294 (6) |
| C12 | 0.3286 (3) | 0.5760 (3) | −0.05311 (18) | 0.0368 (7) |
| C13 | 0.4278 (3) | 0.6647 (3) | −0.0576 (2) | 0.0445 (8) |
| H13 | 0.4398 | 0.6864 | −0.1126 | 0.053* |
| C14 | 0.5061 (3) | 0.7183 (3) | 0.0194 (2) | 0.0472 (8) |
| H14 | 0.5717 | 0.7776 | 0.0171 | 0.057* |
| C15 | 0.4890 (3) | 0.6853 (3) | 0.1024 (2) | 0.0397 (7) |
| H15 | 0.5435 | 0.7237 | 0.1542 | 0.048* |
| C16 | 0.1444 (3) | 0.4307 (3) | −0.11997 (19) | 0.0429 (8) |
| H16 | 0.0881 | 0.3915 | −0.1707 | 0.051* |
| C17 | 0.2384 (3) | 0.5131 (3) | −0.12896 (19) | 0.0453 (8) |
| H17 | 0.2455 | 0.5299 | −0.1859 | 0.054* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0360 (2) | 0.0377 (2) | 0.02556 (18) | 0.00182 (16) | 0.00982 (14) | −0.00183 (15) |
| N1 | 0.0338 (12) | 0.0290 (12) | 0.0281 (11) | 0.0019 (10) | 0.0112 (10) | 0.0016 (9) |
| N2 | 0.0340 (13) | 0.0280 (12) | 0.0336 (12) | 0.0029 (10) | 0.0105 (10) | 0.0010 (10) |
| O1 | 0.0444 (12) | 0.0396 (12) | 0.0349 (11) | 0.0059 (10) | 0.0024 (9) | −0.0066 (9) |
| O2 | 0.0467 (13) | 0.0412 (12) | 0.0381 (11) | 0.0073 (10) | 0.0072 (9) | −0.0055 (9) |
| O3 | 0.0591 (14) | 0.0546 (14) | 0.0325 (11) | 0.0083 (11) | 0.0230 (10) | 0.0053 (10) |
| O4 | 0.095 (2) | 0.0595 (16) | 0.0710 (16) | 0.0257 (15) | 0.0535 (15) | 0.0232 (14) |
| O5 | 0.0495 (12) | 0.0443 (12) | 0.0379 (11) | −0.0074 (10) | 0.0120 (9) | −0.0047 (9) |
| C1 | 0.0351 (15) | 0.0379 (17) | 0.0232 (13) | −0.0013 (13) | 0.0097 (11) | 0.0041 (12) |
| C2 | 0.0365 (16) | 0.0490 (18) | 0.0310 (14) | −0.0073 (14) | 0.0057 (12) | 0.0045 (13) |
| C3 | 0.0428 (17) | 0.0383 (17) | 0.0316 (15) | −0.0051 (13) | 0.0090 (13) | 0.0043 (13) |
| C4 | 0.0410 (17) | 0.0481 (19) | 0.0319 (15) | −0.0069 (14) | 0.0117 (13) | −0.0004 (13) |
| C5 | 0.0417 (17) | 0.0492 (19) | 0.0253 (14) | −0.0065 (15) | 0.0100 (12) | −0.0020 (14) |
| C6 | 0.0390 (16) | 0.0338 (16) | 0.0417 (16) | 0.0031 (13) | 0.0174 (13) | 0.0044 (13) |
| C7 | 0.0359 (16) | 0.0317 (16) | 0.0580 (19) | −0.0016 (13) | 0.0147 (14) | −0.0013 (14) |

| | | | | | |
|---|---|---|---|---|---|
| C8 | 0.0325 (16) | 0.0339 (16) | 0.0475 (18) | 0.0027 (13) | 0.0019 (13) | −0.0101 (14) |
| C9 | 0.0342 (15) | 0.0326 (15) | 0.0313 (14) | 0.0095 (12) | 0.0041 (12) | −0.0017 (12) |
| C10 | 0.0319 (14) | 0.0280 (14) | 0.0274 (13) | 0.0071 (12) | 0.0084 (11) | 0.0002 (11) |
| C11 | 0.0320 (14) | 0.0287 (14) | 0.0287 (14) | 0.0089 (12) | 0.0105 (11) | 0.0026 (11) |
| C12 | 0.0443 (17) | 0.0357 (16) | 0.0342 (15) | 0.0159 (13) | 0.0177 (13) | 0.0100 (12) |
| C13 | 0.0488 (19) | 0.0447 (19) | 0.0476 (18) | 0.0138 (15) | 0.0260 (15) | 0.0163 (15) |
| C14 | 0.0453 (18) | 0.0354 (17) | 0.070 (2) | 0.0027 (14) | 0.0307 (17) | 0.0137 (16) |
| C15 | 0.0370 (16) | 0.0318 (16) | 0.0503 (18) | 0.0004 (13) | 0.0131 (14) | −0.0021 (14) |
| C16 | 0.0475 (18) | 0.0480 (19) | 0.0289 (15) | 0.0103 (15) | 0.0046 (13) | −0.0058 (13) |
| C17 | 0.058 (2) | 0.055 (2) | 0.0246 (15) | 0.0181 (17) | 0.0136 (14) | 0.0054 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O3 | 1.947 (2) | C4—C3[i] | 1.520 (4) |
| Cu1—O1 | 1.9545 (19) | C4—H4A | 0.9700 |
| Cu1—N1 | 2.014 (2) | C4—H4B | 0.9700 |
| Cu1—N2 | 2.022 (2) | C6—C7 | 1.387 (4) |
| Cu1—O5 | 2.385 (2) | C6—H6 | 0.9300 |
| N1—C6 | 1.329 (3) | C7—C8 | 1.362 (4) |
| N1—C10 | 1.360 (3) | C7—H7 | 0.9300 |
| N2—C15 | 1.320 (4) | C8—C9 | 1.404 (4) |
| N2—C11 | 1.362 (3) | C8—H8 | 0.9300 |
| O1—C1 | 1.266 (3) | C9—C10 | 1.401 (4) |
| O2—C1 | 1.243 (3) | C9—C16 | 1.440 (4) |
| O3—C5 | 1.267 (3) | C10—C11 | 1.429 (4) |
| O4—C5 | 1.225 (4) | C11—C12 | 1.402 (4) |
| O5—H51 | 0.8897 | C12—C13 | 1.403 (4) |
| O5—H52 | 0.8804 | C12—C17 | 1.435 (4) |
| C1—C2 | 1.511 (4) | C13—C14 | 1.359 (4) |
| C2—C3 | 1.531 (4) | C13—H13 | 0.9300 |
| C2—H2A | 0.9700 | C14—C15 | 1.401 (4) |
| C2—H2B | 0.9700 | C14—H14 | 0.9300 |
| C3—C4[i] | 1.520 (4) | C15—H15 | 0.9300 |
| C3—H3A | 0.9700 | C16—C17 | 1.340 (5) |
| C3—H3B | 0.9700 | C16—H16 | 0.9300 |
| C4—C5 | 1.518 (4) | C17—H17 | 0.9300 |
| | | | |
| O3—Cu1—O1 | 91.32 (9) | H4A—C4—H4B | 108.2 |
| O3—Cu1—N1 | 91.85 (9) | O4—C5—O3 | 125.6 (3) |
| O1—Cu1—N1 | 165.65 (9) | O4—C5—C4 | 119.0 (3) |
| O3—Cu1—N2 | 173.39 (9) | O3—C5—C4 | 115.3 (3) |
| O1—Cu1—N2 | 94.62 (9) | N1—C6—C7 | 122.6 (3) |
| N1—Cu1—N2 | 81.69 (9) | N1—C6—H6 | 118.7 |
| O3—Cu1—O5 | 99.10 (8) | C7—C6—H6 | 118.7 |
| O1—Cu1—O5 | 95.20 (7) | C8—C7—C6 | 120.0 (3) |
| N1—Cu1—O5 | 98.12 (8) | C8—C7—H7 | 120.0 |
| N2—Cu1—O5 | 83.28 (8) | C6—C7—H7 | 120.0 |
| C6—N1—C10 | 117.9 (2) | C7—C8—C9 | 119.4 (3) |

| | | | |
|---|---|---|---|
| C6—N1—Cu1 | 129.16 (18) | C7—C8—H8 | 120.3 |
| C10—N1—Cu1 | 112.87 (17) | C9—C8—H8 | 120.3 |
| C15—N2—C11 | 117.8 (2) | C10—C9—C8 | 117.3 (3) |
| C15—N2—Cu1 | 129.3 (2) | C10—C9—C16 | 117.9 (3) |
| C11—N2—Cu1 | 112.56 (17) | C8—C9—C16 | 124.8 (3) |
| C1—O1—Cu1 | 108.23 (17) | N1—C10—C9 | 122.8 (2) |
| C5—O3—Cu1 | 125.2 (2) | N1—C10—C11 | 116.4 (2) |
| Cu1—O5—H51 | 91.5 | C9—C10—C11 | 120.7 (2) |
| Cu1—O5—H52 | 113.4 | N2—C11—C12 | 123.6 (3) |
| H51—O5—H52 | 112.2 | N2—C11—C10 | 116.3 (2) |
| O2—C1—O1 | 123.0 (2) | C12—C11—C10 | 120.0 (2) |
| O2—C1—C2 | 120.8 (3) | C11—C12—C13 | 116.9 (3) |
| O1—C1—C2 | 116.1 (3) | C11—C12—C17 | 118.2 (3) |
| C1—C2—C3 | 110.1 (2) | C13—C12—C17 | 124.9 (3) |
| C1—C2—H2A | 109.6 | C14—C13—C12 | 119.0 (3) |
| C3—C2—H2A | 109.6 | C14—C13—H13 | 120.5 |
| C1—C2—H2B | 109.6 | C12—C13—H13 | 120.5 |
| C3—C2—H2B | 109.6 | C13—C14—C15 | 120.7 (3) |
| H2A—C2—H2B | 108.1 | C13—C14—H14 | 119.6 |
| C4$^i$—C3—C2 | 113.5 (2) | C15—C14—H14 | 119.6 |
| C4$^i$—C3—H3A | 108.9 | N2—C15—C14 | 121.9 (3) |
| C2—C3—H3A | 108.9 | N2—C15—H15 | 119.1 |
| C4$^i$—C3—H3B | 108.9 | C14—C15—H15 | 119.1 |
| C2—C3—H3B | 108.9 | C17—C16—C9 | 121.4 (3) |
| H3A—C3—H3B | 107.7 | C17—C16—H16 | 119.3 |
| C5—C4—C3$^i$ | 109.7 (2) | C9—C16—H16 | 119.3 |
| C5—C4—H4A | 109.7 | C16—C17—C12 | 121.8 (3) |
| C3$^i$—C4—H4A | 109.7 | C16—C17—H17 | 119.1 |
| C5—C4—H4B | 109.7 | C12—C17—H17 | 119.1 |
| C3$^i$—C4—H4B | 109.7 | | |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the N1,C6–C10 ring

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H51···O4 | 0.89 | 1.81 | 2.659 (3) | 158 |
| O5—H52···O2$^{ii}$ | 0.88 | 1.89 | 2.762 (3) | 169 |
| C2—H2*A*···*Cg*1$^{ii}$ | 0.97 | 2.88 | 3.754 (3) | 151 |

Symmetry code: (ii) −*x*+1, *y*+1/2, −*z*+1/2.