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# Aquabis(3-chlorobenzoato-κO)bis(*N*,*N*-diethylnicotinamide-κ*N*)copper(II)

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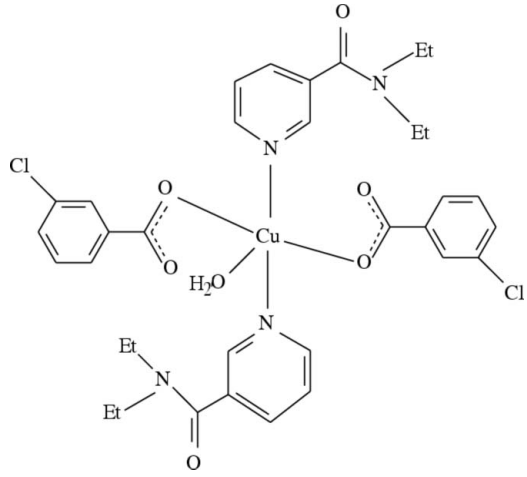
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.032; $wR$ factor = 0.086; data-to-parameter ratio = 27.8.

The title compound, $[Cu(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)]$, has twofold symmetry with the $Cu^{II}$ cation and the O atom of the coordinating water molecule located on the axis. The $Cu^{II}$ cation is coordinated by two carboxylate O atoms of chlorobenzoate (CB) anions, two N atoms of *N*,*N*-diethylnicotinamide (DENA) ligands and one water molecule in a distorted $N_2O_3$ square-pyramidal geometry. The benzene and pyridine rings are oriented at a dihedral angle of 82.51 (6)°. In the anionic ligand, the carboxylate group is twisted away from the attached benzene ring by 12.85 (11)°. In the crystal, O—H···O hydrogen bonds between the coordinating water molecule and the carboxyl group link the complex molecules into supramolecular chains running along the *c*-axis direction.

## Related literature

For literature on niacin, see: Krishnamachari (1974). For information on the nicotinic acid derivative *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a*,*b*); Hökelek & Necefoğlu (1998, 2007); Necefoğlu *et al.* (2011*a*,*b*,*c*). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$[Cu(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)]$
$M_r$ = 749.13
Orthorhombic, *Iba*2
$a$ = 15.9185 (9) Å
$b$ = 19.2366 (11) Å
$c$ = 11.5535 (7) Å
$V$ = 3537.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.82 mm$^{-1}$
$T$ = 296 K
0.35 × 0.20 × 0.15 mm

### Data collection

Bruker SMART BREEZE CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min}$ = 0.821, $T_{max}$ = 0.884
75834 measured reflections
6232 independent reflections
5189 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
$S$ = 1.06
6232 reflections
224 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$
Absolute structure: Flack (1983), with no Friedel pairs measured
Flack parameter: 0.027 (10)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.0294 (12) | Cu1—O4 | 2.238 (2) |
| Cu1—O1 | 1.9337 (10) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H41···O2$^{i}$ | 0.79 (4) | 1.95 (3) | 2.7367 (17) | 171 (4) |

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics:

*ORTEP-3* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5719).

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# supporting information

*Acta Cryst.* (2013). E**69**, m458–m459 [doi:10.1107/S1600536813018989]

## Aquabis(3-chlorobenzoato-$\kappa O$)bis(*N*,*N*-diethylnicotinamide-$\kappa N$)copper(II)

**Nihat Bozkurt, Tuncay Tunç, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek**

### S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title mononuclear $Cu^{II}$ complex, (Fig. 1), contains one-half molecule, the $Cu^{II}$ cation is located on a twofold rotation axis and is coordinated by carboxylate O atoms of two chlorobenzoate (CB) anions, N atoms of two *N*,*N*-diethylnicotinamide (DENA) ligands and by one water molecule, located on a twofold rotation axis, all ligands coordinating in a monodentate manner. The crystal structures of similar complexes of $Cu^{II}$, $Co^{II}$, $Ni^{II}$, $Mn^{II}$ and $Zn^{II}$ cations, $[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_2O)_2]$ (Hökelek *et al.*, 1996); $[Cu(C_9H_9O_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$ (Necefoğlu *et al.*, 2011*a*); $[Cu(C_7H_4FO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$ (Necefoğlu *et al.*, 2011*b*); $[Co(C_6H_6N_2O)_2(C_7H_4NO_4)_2(H_2O)_2]$ (Hökelek & Necefoğlu, 1998); $[Co(C_9H_9O_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$ (Necefoğlu *et al.*, 2011*c*); $[Ni(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*a*); $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2H_2O$ (Hökelek & Necefoğlu, 2007) and $[Zn(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*b*) have also been reported. In the first copper(II) complex mentioned above the two benzoate ions coordinate to the $Cu^{II}$ atom as bidentate ligands, while in the other structures all the ligands coordinate in a monodentate manner.

In the title complex, the four symmetry related O and N atoms (O1, O1a and N1, N1a) [symmetry code: (a) - *x*, 1 - *y*, *z*] in the equatorial plane around the $Cu^{II}$ cation form a distorted square-planar arrangement, while the distorted square-pyramidal coordination is completed by the water O atom (O4) in the axial position.

The Cu—O bond lengths are 1.9346 (11) Å (for benzoate oxygen) and 2.238 (2) Å (for water oxygen), and the Cu—N bond length is 2.0303 (14) Å, close to standard values (Allen *et al.*, 1987). The Cu atom is displaced out of the mean-plane of the carboxylate group (O1/C1/O2) by -0.1606 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring *A* (C2—C7) is 12.85 (11)°. The benzene *A* (C2—C7) and the pyridine *B* (N1/C8—C12) rings are oriented at a dihedral angle of 82.51 (6)°.

In the crystal, strong O—H···O hydrogen bonds (Table 2) link the water hydrogens to the carboxylate oxygens into infinite chains along the c-axis.

### S2. Experimental

The title compound was prepared by the reaction of $CuSO_4.5H_2O$ (1.25 g, 5 mmol) in $H_2O$ (100 ml) and diethyl-nicotinamide (1.78 g, 10 mmol) in $H_2O$ (20 ml) with sodium 3-chlorobenzoate (1.79 g, 10 mmol) in $H_2O$ (100 ml). The mixture was set aside to crystallize at ambient temperature for five days, giving blue single crystals.

### S3. Refinement

Atom H41 (for $H_2O$) was located in a difference Fourier map and was refined freely. The C-bound H-atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H-atoms, respectively,

and constrained to ride on their parent atoms, with $U_{iso}$(H) = k × $U_{eq}$(C), where k = 1.5 for methyl H-atoms and k = 1.2 for all other H-atoms.

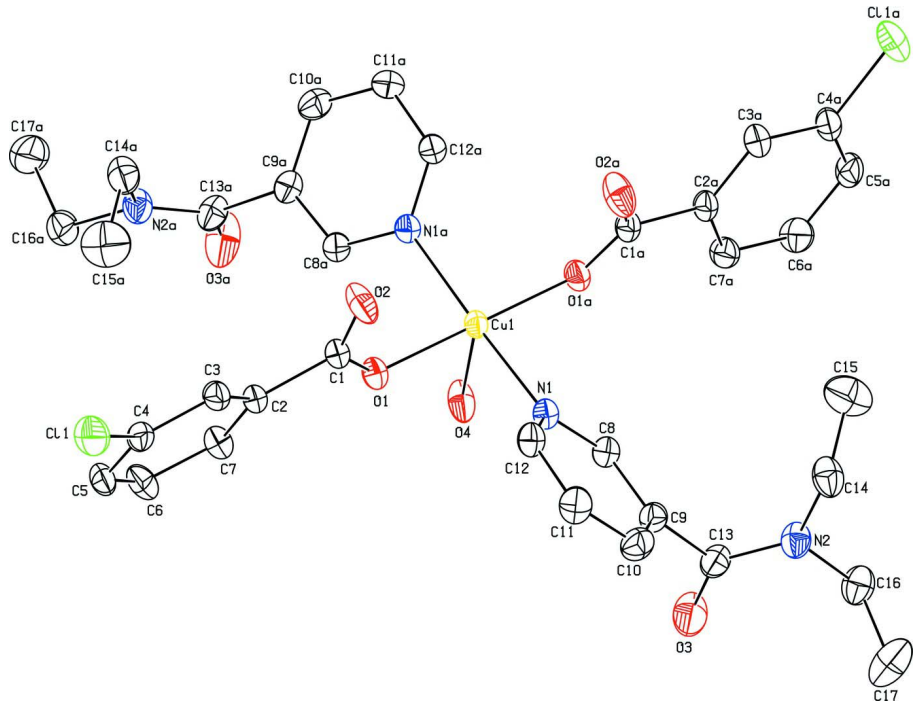


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (a) 2 - *x*, 1 - *y*, *z*]. Hydrogen atoms have been omitted for clarity.

**Aquabis(3-chlorobenzoato-*κO*)bis(*N*,*N*-diethylnicotinamide-*κN*)copper(II)**

*Crystal data*

$[Cu(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)]$
$M_r$ = 749.13
Orthorhombic, *Iba*2
Hall symbol: I 2 -2c
*a* = 15.9185 (9) Å
*b* = 19.2366 (11) Å
*c* = 11.5535 (7) Å
*V* = 3537.9 (4) Å$^3$
*Z* = 4
*F*(000) = 1556
$D_x$ = 1.406 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9278 reflections
*θ* = 2.2–30.7°
*μ* = 0.82 mm$^{-1}$
*T* = 296 K
Block, blue
0.35 × 0.20 × 0.15 mm

*Data collection*

Bruker SMART BREEZE CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
*φ* and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min}$ = 0.821, $T_{max}$ = 0.884
75834 measured reflections
6232 independent reflections
5189 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 32.3°, $\theta_{min}$ = 1.7°
*h* = −23→23
*k* = −28→28
*l* = −17→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.06$
6232 reflections
224 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.4582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{min} = -0.39$ e Å$^{-3}$
Absolute structure: Flack (1983), with no Friedel pairs measured
Absolute structure parameter: 0.027 (10)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 | 1.0000 | 0.5000 | 0.41873 (3) | 0.03000 (6) |
| Cl1 | 1.46828 (3) | 0.59979 (3) | 0.63513 (5) | 0.06445 (15) |
| O1 | 1.11786 (6) | 0.52434 (6) | 0.41852 (13) | 0.0393 (2) |
| O2 | 1.14688 (8) | 0.52348 (10) | 0.60832 (13) | 0.0614 (4) |
| O3 | 0.84439 (11) | 0.72659 (11) | 0.16031 (16) | 0.0800 (5) |
| O4 | 1.0000 | 0.5000 | 0.22505 (18) | 0.0538 (6) |
| H41 | 1.0395 (19) | 0.4937 (15) | 0.185 (4) | 0.083 (10)* |
| N1 | 0.96843 (7) | 0.60210 (6) | 0.42656 (14) | 0.0353 (2) |
| N2 | 0.74305 (10) | 0.72799 (9) | 0.29566 (14) | 0.0469 (3) |
| C1 | 1.16668 (9) | 0.52875 (9) | 0.50510 (15) | 0.0363 (3) |
| C2 | 1.25768 (9) | 0.54254 (8) | 0.47400 (14) | 0.0349 (3) |
| C3 | 1.31396 (9) | 0.56202 (9) | 0.56019 (15) | 0.0391 (3) |
| H3 | 1.2964 | 0.5673 | 0.6364 | 0.047* |
| C4 | 1.39704 (10) | 0.57329 (8) | 0.52927 (16) | 0.0414 (3) |
| C5 | 1.42506 (9) | 0.56541 (8) | 0.4176 (2) | 0.0469 (3) |
| H5 | 1.4812 | 0.5729 | 0.3992 | 0.056* |
| C6 | 1.36773 (12) | 0.54600 (10) | 0.33236 (19) | 0.0514 (4) |
| H6 | 1.3857 | 0.5403 | 0.2563 | 0.062* |
| C7 | 1.28426 (11) | 0.53510 (9) | 0.36030 (17) | 0.0422 (4) |
| H7 | 1.2460 | 0.5228 | 0.3030 | 0.051* |
| C8 | 0.90811 (10) | 0.62540 (8) | 0.35534 (15) | 0.0372 (3) |
| H8 | 0.8802 | 0.5936 | 0.3084 | 0.045* |
| C9 | 0.88569 (10) | 0.69476 (8) | 0.34881 (14) | 0.0398 (3) |

| | | | | |
|---|---|---|---|---|
| C10 | 0.92796 (12) | 0.74174 (8) | 0.4190 (2) | 0.0510 (4) |
| H10 | 0.9146 | 0.7888 | 0.4161 | 0.061* |
| C11 | 0.99002 (12) | 0.71828 (10) | 0.4931 (2) | 0.0509 (4) |
| H11 | 1.0188 | 0.7490 | 0.5409 | 0.061* |
| C12 | 1.00827 (10) | 0.64755 (10) | 0.49440 (18) | 0.0412 (3) |
| H12 | 1.0497 | 0.6314 | 0.5443 | 0.049* |
| C13 | 0.82193 (13) | 0.71794 (10) | 0.26044 (15) | 0.0462 (4) |
| C14 | 0.71426 (12) | 0.71772 (12) | 0.4142 (2) | 0.0551 (4) |
| H14A | 0.6784 | 0.7563 | 0.4361 | 0.066* |
| H14B | 0.7625 | 0.7177 | 0.4656 | 0.066* |
| C15 | 0.6667 (2) | 0.65112 (17) | 0.4298 (3) | 0.0907 (8) |
| H15A | 0.6454 | 0.6486 | 0.5074 | 0.136* |
| H15B | 0.7036 | 0.6125 | 0.4159 | 0.136* |
| H15C | 0.6208 | 0.6496 | 0.3760 | 0.136* |
| C16 | 0.68061 (14) | 0.75374 (11) | 0.2115 (2) | 0.0546 (5) |
| H16A | 0.6255 | 0.7363 | 0.2325 | 0.066* |
| H16B | 0.6943 | 0.7358 | 0.1353 | 0.066* |
| C17 | 0.6778 (2) | 0.83180 (13) | 0.2067 (3) | 0.0864 (9) |
| H17A | 0.6405 | 0.8462 | 0.1461 | 0.130* |
| H17B | 0.7332 | 0.8495 | 0.1916 | 0.130* |
| H17C | 0.6581 | 0.8496 | 0.2795 | 0.130* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.02380 (9) | 0.03532 (10) | 0.03087 (11) | 0.00119 (8) | 0.000 | 0.000 |
| Cl1 | 0.0404 (2) | 0.0777 (3) | 0.0752 (4) | −0.0116 (2) | −0.0184 (2) | 0.0065 (3) |
| O1 | 0.0265 (4) | 0.0465 (5) | 0.0449 (5) | −0.0019 (4) | −0.0005 (5) | −0.0018 (7) |
| O2 | 0.0334 (6) | 0.1087 (12) | 0.0420 (7) | −0.0084 (7) | 0.0062 (5) | 0.0074 (8) |
| O3 | 0.0700 (10) | 0.1258 (14) | 0.0442 (8) | 0.0380 (10) | 0.0141 (8) | 0.0253 (10) |
| O4 | 0.0329 (9) | 0.1020 (18) | 0.0265 (10) | 0.0133 (9) | 0.000 | 0.000 |
| N1 | 0.0290 (5) | 0.0383 (5) | 0.0385 (7) | 0.0010 (4) | 0.0002 (6) | −0.0028 (6) |
| N2 | 0.0421 (7) | 0.0617 (8) | 0.0369 (7) | 0.0086 (6) | −0.0025 (6) | −0.0013 (7) |
| C1 | 0.0271 (6) | 0.0404 (8) | 0.0414 (8) | 0.0011 (5) | 0.0034 (5) | 0.0022 (6) |
| C2 | 0.0259 (6) | 0.0380 (7) | 0.0408 (8) | 0.0008 (5) | 0.0023 (6) | 0.0036 (6) |
| C3 | 0.0304 (6) | 0.0462 (8) | 0.0409 (8) | −0.0006 (6) | −0.0011 (6) | 0.0060 (6) |
| C4 | 0.0292 (6) | 0.0394 (7) | 0.0556 (10) | −0.0005 (6) | −0.0050 (6) | 0.0073 (7) |
| C5 | 0.0283 (6) | 0.0440 (7) | 0.0683 (10) | −0.0026 (5) | 0.0105 (8) | 0.0012 (10) |
| C6 | 0.0425 (9) | 0.0593 (10) | 0.0523 (11) | −0.0073 (7) | 0.0181 (8) | −0.0060 (8) |
| C7 | 0.0353 (7) | 0.0488 (9) | 0.0426 (9) | −0.0033 (6) | 0.0052 (7) | −0.0042 (7) |
| C8 | 0.0340 (7) | 0.0392 (7) | 0.0385 (8) | 0.0023 (5) | −0.0017 (6) | −0.0016 (6) |
| C9 | 0.0390 (7) | 0.0417 (7) | 0.0389 (8) | 0.0065 (6) | 0.0043 (6) | 0.0030 (6) |
| C10 | 0.0548 (9) | 0.0352 (6) | 0.0631 (10) | 0.0041 (6) | 0.0000 (11) | −0.0029 (10) |
| C11 | 0.0458 (9) | 0.0426 (9) | 0.0643 (12) | −0.0027 (7) | −0.0054 (8) | −0.0141 (8) |
| C12 | 0.0339 (7) | 0.0463 (8) | 0.0435 (9) | 0.0026 (6) | −0.0029 (6) | −0.0071 (7) |
| C13 | 0.0503 (9) | 0.0505 (9) | 0.0377 (9) | 0.0151 (8) | 0.0031 (7) | 0.0035 (7) |
| C14 | 0.0438 (8) | 0.0812 (12) | 0.0405 (8) | 0.0058 (8) | 0.0010 (9) | −0.0060 (12) |
| C15 | 0.099 (2) | 0.0903 (18) | 0.0825 (19) | −0.0149 (15) | 0.0178 (19) | 0.0077 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0501 (10) | 0.0630 (11) | 0.0508 (10) | 0.0082 (8) | −0.0108 (8) | −0.0045 (9) |
| C17 | 0.094 (2) | 0.0615 (13) | 0.104 (2) | 0.0226 (13) | −0.0383 (17) | −0.0114 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.0294 (12) | C7—H7 | 0.9300 |
| Cu1—N1$^{i}$ | 2.0294 (12) | C8—H8 | 0.9300 |
| Cu1—O1 | 1.9337 (10) | C9—C8 | 1.383 (2) |
| Cu1—O1$^{i}$ | 1.9337 (10) | C9—C10 | 1.388 (3) |
| Cu1—O4 | 2.238 (2) | C9—C13 | 1.507 (2) |
| Cl1—C4 | 1.7439 (18) | C10—C11 | 1.383 (3) |
| O1—C1 | 1.269 (2) | C10—H10 | 0.9300 |
| O4—H41 | 0.79 (4) | C11—H11 | 0.9300 |
| N1—C8 | 1.341 (2) | C12—C11 | 1.391 (3) |
| N1—C12 | 1.335 (2) | C12—H12 | 0.9300 |
| N2—C13 | 1.334 (2) | C13—O3 | 1.222 (2) |
| N2—C14 | 1.458 (3) | C14—C15 | 1.499 (4) |
| N2—C16 | 1.476 (3) | C14—H14A | 0.9700 |
| C1—O2 | 1.238 (2) | C14—H14B | 0.9700 |
| C1—C2 | 1.516 (2) | C15—H15A | 0.9600 |
| C2—C3 | 1.391 (2) | C15—H15B | 0.9600 |
| C2—C7 | 1.387 (2) | C15—H15C | 0.9600 |
| C3—C4 | 1.387 (2) | C16—C17 | 1.503 (3) |
| C3—H3 | 0.9300 | C16—H16A | 0.9700 |
| C5—C4 | 1.373 (3) | C16—H16B | 0.9700 |
| C5—C6 | 1.394 (3) | C17—H17A | 0.9600 |
| C5—H5 | 0.9300 | C17—H17B | 0.9600 |
| C6—H6 | 0.9300 | C17—H17C | 0.9600 |
| C7—C6 | 1.383 (2) | | |

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| O1—Cu1—O1$^{i}$ | 179.86 (9) | C9—C8—H8 | 118.6 |
| O1—Cu1—O4 | 89.93 (5) | C8—C9—C10 | 118.11 (16) |
| O1$^{i}$—Cu1—O4 | 89.93 (5) | C8—C9—C13 | 119.75 (16) |
| O1—Cu1—N1 | 90.35 (5) | C10—C9—C13 | 121.96 (15) |
| O1$^{i}$—Cu1—N1 | 89.66 (5) | C9—C10—H10 | 120.2 |
| O1—Cu1—N1$^{i}$ | 89.66 (5) | C11—C10—C9 | 119.69 (15) |
| O1$^{i}$—Cu1—N1$^{i}$ | 90.35 (5) | C11—C10—H10 | 120.2 |
| N1—Cu1—O4 | 92.55 (5) | C10—C11—C12 | 118.36 (17) |
| N1$^{i}$—Cu1—O4 | 92.55 (5) | C10—C11—H11 | 120.8 |
| N1$^{i}$—Cu1—N1 | 174.89 (9) | C12—C11—H11 | 120.8 |
| C1—O1—Cu1 | 127.53 (12) | N1—C12—C11 | 122.34 (17) |
| Cu1—O4—H41 | 126 (3) | N1—C12—H12 | 118.8 |
| C8—N1—Cu1 | 118.25 (11) | C11—C12—H12 | 118.8 |
| C12—N1—Cu1 | 122.85 (12) | O3—C13—N2 | 122.97 (18) |
| C12—N1—C8 | 118.79 (13) | O3—C13—C9 | 118.98 (17) |
| C13—N2—C14 | 124.25 (16) | N2—C13—C9 | 118.05 (16) |
| C13—N2—C16 | 118.78 (16) | N2—C14—C15 | 112.8 (2) |
| C14—N2—C16 | 116.93 (15) | N2—C14—H14A | 109.0 |

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| O1—C1—C2 | 114.20 (14) | N2—C14—H14B | 109.0 |
| O2—C1—O1 | 126.72 (15) | C15—C14—H14A | 109.0 |
| O2—C1—C2 | 119.08 (15) | C15—C14—H14B | 109.0 |
| C3—C2—C1 | 119.53 (15) | H14A—C14—H14B | 107.8 |
| C7—C2—C1 | 119.85 (14) | C14—C15—H15A | 109.5 |
| C7—C2—C3 | 120.62 (14) | C14—C15—H15B | 109.5 |
| C2—C3—H3 | 120.9 | C14—C15—H15C | 109.5 |
| C4—C3—C2 | 118.15 (16) | H15A—C15—H15B | 109.5 |
| C4—C3—H3 | 120.9 | H15A—C15—H15C | 109.5 |
| C3—C4—Cl1 | 119.02 (14) | H15B—C15—H15C | 109.5 |
| C5—C4—Cl1 | 118.68 (12) | N2—C16—C17 | 112.26 (19) |
| C5—C4—C3 | 122.30 (16) | N2—C16—H16A | 109.2 |
| C4—C5—C6 | 118.74 (14) | N2—C16—H16B | 109.2 |
| C4—C5—H5 | 120.6 | C17—C16—H16A | 109.2 |
| C6—C5—H5 | 120.6 | C17—C16—H16B | 109.2 |
| C5—C6—H6 | 119.8 | H16A—C16—H16B | 107.9 |
| C7—C6—C5 | 120.31 (18) | C16—C17—H17A | 109.5 |
| C7—C6—H6 | 119.8 | C16—C17—H17B | 109.5 |
| C2—C7—H7 | 120.1 | C16—C17—H17C | 109.5 |
| C6—C7—C2 | 119.87 (17) | H17A—C17—H17B | 109.5 |
| C6—C7—H7 | 120.1 | H17A—C17—H17C | 109.5 |
| N1—C8—C9 | 122.71 (15) | H17B—C17—H17C | 109.5 |
| N1—C8—H8 | 118.6 | | |

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| O4—Cu1—O1—C1 | −173.97 (13) | O1—C1—C2—C7 | −13.2 (2) |
| N1—Cu1—O1—C1 | 93.48 (14) | O2—C1—C2—C3 | −12.1 (2) |
| N1$^{i}$—Cu1—O1—C1 | −81.41 (14) | O2—C1—C2—C7 | 167.34 (19) |
| O1—Cu1—N1—C8 | 133.82 (13) | C1—C2—C3—C4 | 179.08 (15) |
| O1$^{i}$—Cu1—N1—C8 | −46.04 (13) | C7—C2—C3—C4 | −0.4 (2) |
| O1—Cu1—N1—C12 | −42.21 (15) | C1—C2—C7—C6 | −178.40 (16) |
| O1$^{i}$—Cu1—N1—C12 | 137.94 (15) | C3—C2—C7—C6 | 1.1 (3) |
| O4—Cu1—N1—C8 | 43.87 (12) | C2—C3—C4—Cl1 | 178.47 (12) |
| O4—Cu1—N1—C12 | −132.15 (14) | C2—C3—C4—C5 | −0.4 (2) |
| Cu1—O1—C1—O2 | −6.0 (3) | C6—C5—C4—Cl1 | −178.34 (14) |
| Cu1—O1—C1—C2 | 174.59 (9) | C6—C5—C4—C3 | 0.6 (3) |
| Cu1—N1—C8—C9 | −175.86 (13) | C4—C5—C6—C7 | 0.1 (3) |
| C12—N1—C8—C9 | 0.3 (3) | C2—C7—C6—C5 | −0.9 (3) |
| Cu1—N1—C12—C11 | 175.38 (16) | C10—C9—C8—N1 | 0.2 (3) |
| C8—N1—C12—C11 | −0.6 (3) | C13—C9—C8—N1 | 175.42 (16) |
| C14—N2—C13—O3 | 179.6 (2) | C8—C9—C10—C11 | −0.5 (3) |
| C14—N2—C13—C9 | −0.3 (3) | C13—C9—C10—C11 | −175.56 (19) |
| C16—N2—C13—O3 | −2.8 (3) | C8—C9—C13—O3 | −79.9 (3) |
| C16—N2—C13—C9 | 177.28 (16) | C8—C9—C13—N2 | 100.0 (2) |
| C13—N2—C14—C15 | −102.9 (3) | C10—C9—C13—O3 | 95.1 (3) |
| C16—N2—C14—C15 | 79.5 (3) | C10—C9—C13—N2 | −85.0 (2) |
| C13—N2—C16—C17 | −88.5 (3) | C9—C10—C11—C12 | 0.2 (3) |

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| C14—N2—C16—C17 | 89.2 (3) | N1—C12—C11—C10 | 0.4 (3) |
| O1—C1—C2—C3 | 167.34 (15) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H41···O2$^{ii}$ | 0.79 (4) | 1.95 (3) | 2.7367 (17) | 171 (4) |

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