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# μ-1,6-Dioxo-1,6-diphenylhexane-3,4-diolato-bis[(2,2'-bipyridine)chloridocopper(II)] dihydrate a; b; a

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IUCrData

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# μ-1,6-Dioxo-1,6-diphenylhexane-3,4-diolato-bis[(2,2′-bipyridine)chloridocopper(II)] dihydrate

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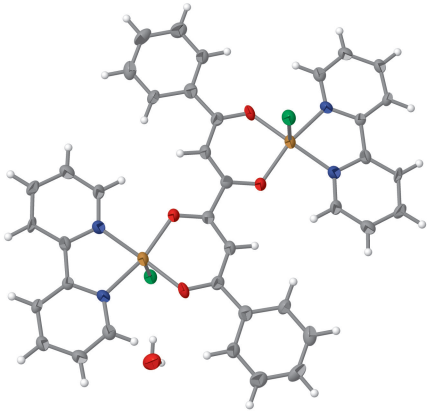
**Keywords:** $Cu^{II}$; hydrate; hydrogen-bonding; tetronedioate; crystal structure.

**CCDC reference:** 2288356

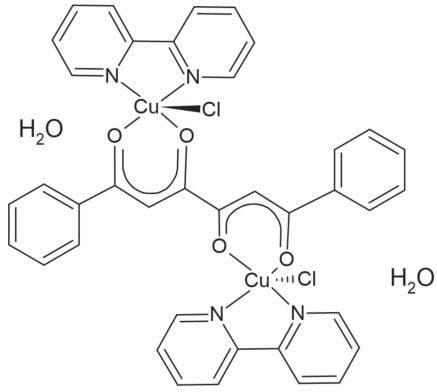
**Structural data:** full structural data are available from iucrdata.iucr.org

The reaction of $CuCl_2$ with 1,6-diphenyl-1,3,5,6-hexanetetrone and 2,2′-bipyridine (bipy) in ethanol gave crystals of the corresponding bimetallic complex, $[Cu_2(C_{18}H_{12}O_4)Cl_2(C_{10}H_8N_2)_2]\cdot 2H_2O$. The molecule is centrosymmetric with each $Cu^{II}$ ion coordinated to two oxygen atoms from the tetronediate, two nitrogen atoms from a bipy ligand and one coordinated chloride ion. A water molecule of crystallization forms hydrogen bonds to the chloride ions, linking the molecules into a chain parallel to the *bc*-face diagonal.

3D view



Chemical scheme




## Structure description

1,6-Diphenyl-1,3,4,6-hexanetetrone has been known for over 100 years (Widman & Virgin, 1909) and its structure has been reported (Kaitner *et al.*, 1992). Both its synthesis by oxidation (Balenović *et al.*, 1954) and its reactions with oxidizing agents have been studied (Balenović, 1948; Bird & Thorley, 1977; Poje *et al.*, 1978), as well as its use as a starting material for the preparation of a variety of aminated products (Lacan *et al.*, 1973; Unterhalt & Pindur, 1977; Kaitner *et al.*, 1992; Waring *et al.*, 2002; Kobelev *et al.*, 2019). The backbone core resembles a bis-acac structure and and as such it has been used in the preparation of transition-metal complexes (Boucher & Bailar, 1964; Saalfrank *et al.*, 1998; Nawar, 1994). However, we were surprised to find that there are no reported structures of transition-metal complexes containing this ligand (Groom *et al.*, 2016). We investigated its coordination chemistry with $Cu^{II}$ as part of our studies on potential magnetic ladders (Monroe *et al.*, 2022).

The molecule sits astride a crystallographic inversion center (Fig. 1). Each $Cu^{II}$ ion is five-coordinate, including two oxygen atoms from the tetronediate ligand, two nitrogen atoms from a bipy molecule and one coordinated chloride ion. The $CuN_2O_2$ equatorial plane is nearly planar (mean deviation of the $N_2O_2$ donor set = 0.0219 Å) with the $Cu^{II}$ ion displaced [0.2219 (15) Å] toward the chloride ion. The 1,3-dionato motif chelates a

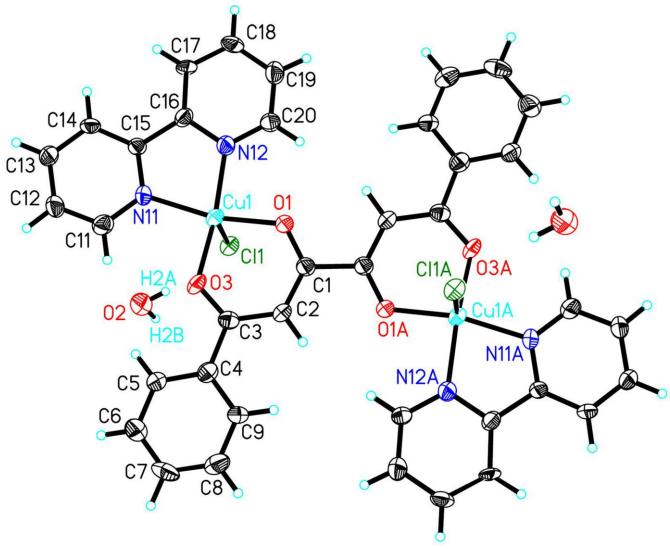



**Figure 1**
The molecular structure of the title compound. Only the asymmetric unit and Cu coordination spheres are labeled. Hydrogen atoms are shown as spheres of arbitrary size. Symmetry operation B: $-x, 1-y, 2-z$.

copper ion and generates a six-membered metallocyclic ring that is only slightly less planar (mean deviation of constituent atoms = 0.1207 Å). The two heterocyclic rings are co-planar as required by symmetry. The pyridyl rings are canted 0.67 (13)° from each other.

$\pi$-Stacking is observed between molecules. The Cu1-dionato ring sits above the N11-containing bpy ring with an interplanar distance of 3.33 (2) Å; the rings are canted 4.4 (2)° with respect to each other. The distance between the ring centroids is 3.73 (2) Å with a slip angle of 25.1 (3)°. This effectively blocks the vacant coordination site on Cu1, preventing the addition of a sixth ligand. $\pi$-Stacking is also observed between the phenyl rings of the tetrone ligand. Adjacent phenyl rings are parallel with an interplanar distance of 3.33 (2) Å with a slip angle of 22.8 (3)°. The bimetallic units are linked into chains *via* hydrogen bonds between the solvent water molecules and chloride ions (Table 1 and Fig. 2).

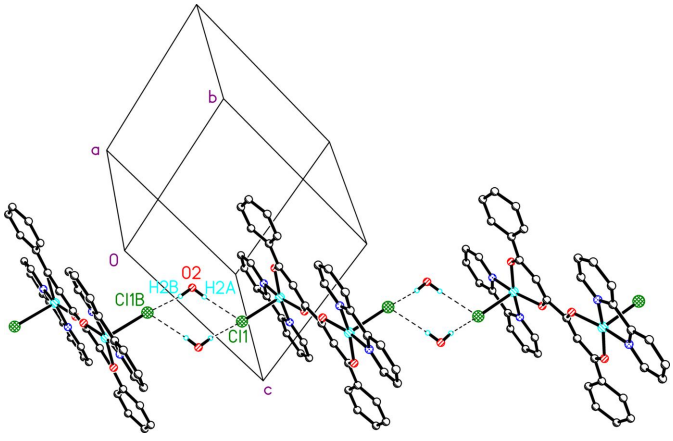



**Figure 2**
Chain formation *via* hydrogen bonding. Symmetry operation B: $-x, -y, 1-z$.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2$A$···Cl1 | 0.82 (5) | 2.41 (5) | 3.224 (3) | 171 (5) |
| O2—H2$B$···Cl1$^{i}$ | 0.98 (4) | 2.33 (5) | 3.307 (4) | 172 (4) |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cu_2(C_{18}H_{12}O_4)Cl_2(C_{10}H_8N_2)_2]\cdot 2H_2O$ |
| $M_r$ | 838.65 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 123 |
| $a, b, c$ (Å) | 8.7211 (2), 10.4194 (2), 10.5243 (7) |
| $\alpha, \beta, \gamma$ (°) | 106.426 (7), 109.090 (8), 90.373 (6) |
| $V$ (Å$^3$) | 861.67 (8) |
| $Z$ | 1 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.41 |
| Crystal size (mm) | 0.13 × 0.09 × 0.02 |
| | |
| Data collection | |
| Diffractometer | Rigaku Spider |
| Absorption correction | Multi-scan (*ABSCOR*; Rigaku, 1995) |
| $T_{min}$, $T_{max}$ | 0.641, 0.929 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 7470, 2552, 1901 |
| $R_{int}$ | 0.046 |
| $\theta_{max}$ (°) | 61.1 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.568 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.047, 0.121, 1.13 |
| No. of reflections | 2552 |
| No. of parameters | 241 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.57, −0.49 |

Computer programs: *CrystalClear* (Rigaku, 2005), *PROCESS-AUTO* (Rigaku, 1998), *SHELXS97* (Sheldrick, 2008), and *SHELXL2018/3* (Sheldrick, 2015), *XP* (Sheldrick, 2008).

## Synthesis and crystallization

$CuCl_2$ (0.403 g, 2.99 mmol) was dissolved in 50 ml of absolute ethanol to generate a green solution. 2,2′-Bipyridine (0.469 g, 3.01 mmol) was added to the solution with stirring to make a light-blue slurry. Addition of 1,6-diphenyl-1,3,4,6-hexanetetrone (0.438 g, 1.49 mmol) generated a lime green slurry, which was stirred for 1 h. The precipitate was recovered by vacuum filtration, washed with ethanol and dried in air to yield 0.973 g of lime green powder (77%). Crystals suitable for X-ray diffraction were grown by recrystallization from DMF.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Eight reflections were omitted from the final refinement owing to poor agreement; details are included in the CIF.

## Acknowledgements

LN is grateful for a Murdock Summer Research Fellowship. Author contributions: LN (synthesis, characterization) JLW (X-ray data) MMT (concept, writing).

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# full crystallographic data

*IUCrData* (2023). **8**, x230713 [https://doi.org/10.1107/S2414314623007137]

## $\mu$-1,6-Dioxo-1,6-diphenylhexane-3,4-diolato-bis[(2,2′-bipyridine)-chloridocopper(II)] dihydrate

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### $\mu$-1,6-Dioxo-1,6-diphenylhexane-3,4-diolato-bis[(2,2′-bipyridine)chloridocopper(II)] dihydrate

*Crystal data*

$[Cu_2(C_{18}H_{12}O_4)Cl_2(C_{10}H_8N_2)_2]\cdot 2H_2O$
$M_r$ = 838.65
Triclinic, $P\overline{1}$
$a$ = 8.7211 (2) Å
$b$ = 10.4194 (2) Å
$c$ = 10.5243 (7) Å
$\alpha$ = 106.426 (7)°
$\beta$ = 109.090 (8)°
$\gamma$ = 90.373 (6)°
$V$ = 861.67 (8) Å$^3$
$Z$ = 1
$F(000)$ = 428
$D_x$ = 1.616 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 3450 reflections
$\theta$ = 6.6–72.0°
$\mu$ = 3.41 mm$^{-1}$
$T$ = 123 K
Plate, green
0.13 × 0.09 × 0.02 mm

*Data collection*

Rigaku Spider diffractometer
Radiation source: rotating anode
Confocal optics monochromator
Detector resolution: 10 pixels mm$^{-1}$
$\omega$–scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
$T_{min}$ = 0.641, $T_{max}$ = 0.929
7470 measured reflections
2552 independent reflections
1901 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046
$\theta_{max}$ = 61.1°, $\theta_{min}$ = 6.6°
$h$ = −9→9
$k$ = −8→11
$l$ = −11→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.121
$S$ = 1.13
2552 reflections
241 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.1469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.49 e Å$^{-3}$

*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**. Hydrogen atoms bonded to carbon atoms were placed geometrically and refined with fixed isotropic thermal parameters. Hydrogen atoms bonded to O2 were located in the difference map and their positions refined with fixed isotropic thermal parameters (O—H = 0.82 (5) & 0.98 (4) Å).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.33000 (7) | 0.32164 (6) | 0.96525 (6) | 0.0307 (2) |
| Cl1 | 0.11639 (12) | 0.13154 (10) | 0.77171 (10) | 0.0345 (3) |
| O1 | 0.1754 (3) | 0.4177 (3) | 1.0408 (3) | 0.0324 (7) |
| C1 | 0.0704 (5) | 0.4796 (4) | 0.9723 (4) | 0.0254 (10) |
| C2 | 0.0728 (5) | 0.5143 (4) | 0.8569 (4) | 0.0294 (10) |
| H2 | −0.017613 | 0.555390 | 0.812000 | 0.035* |
| O3 | 0.3211 (3) | 0.4301 (3) | 0.8421 (3) | 0.0330 (7) |
| C3 | 0.2001 (5) | 0.4937 (4) | 0.7987 (4) | 0.0271 (10) |
| C4 | 0.1975 (5) | 0.5506 (4) | 0.6837 (4) | 0.0303 (10) |
| C5 | 0.2992 (5) | 0.5074 (4) | 0.6059 (4) | 0.0329 (11) |
| H5 | 0.372026 | 0.443341 | 0.628745 | 0.039* |
| C6 | 0.2963 (5) | 0.5555 (5) | 0.4963 (5) | 0.0411 (12) |
| H6 | 0.365425 | 0.523306 | 0.443454 | 0.049* |
| C7 | 0.1939 (6) | 0.6503 (5) | 0.4627 (5) | 0.0422 (12) |
| H7 | 0.193055 | 0.683511 | 0.387222 | 0.051* |
| C8 | 0.0922 (5) | 0.6969 (4) | 0.5389 (5) | 0.0393 (12) |
| H8 | 0.022438 | 0.763064 | 0.516788 | 0.047* |
| C9 | 0.0926 (5) | 0.6469 (4) | 0.6470 (4) | 0.0310 (10) |
| H9 | 0.020939 | 0.677797 | 0.697730 | 0.037* |
| N11 | 0.5341 (4) | 0.2451 (3) | 0.9445 (3) | 0.0282 (8) |
| C11 | 0.6014 (5) | 0.2564 (4) | 0.8501 (4) | 0.0339 (11) |
| H11 | 0.549680 | 0.303493 | 0.785150 | 0.041* |
| C12 | 0.7425 (5) | 0.2020 (4) | 0.8441 (4) | 0.0343 (11) |
| H12 | 0.788780 | 0.212980 | 0.777127 | 0.041* |
| C13 | 0.8170 (5) | 0.1309 (4) | 0.9368 (4) | 0.0302 (10) |
| H13 | 0.914522 | 0.092053 | 0.933922 | 0.036* |
| C14 | 0.7475 (5) | 0.1177 (4) | 1.0326 (4) | 0.0277 (10) |
| H14 | 0.796296 | 0.069566 | 1.097313 | 0.033* |
| C15 | 0.6054 (5) | 0.1754 (4) | 1.0339 (4) | 0.0237 (9) |
| C16 | 0.5227 (5) | 0.1699 (4) | 1.1351 (4) | 0.0275 (10) |
| C17 | 0.5733 (5) | 0.1040 (4) | 1.2364 (4) | 0.0273 (10) |
| H17 | 0.667767 | 0.057482 | 1.244906 | 0.033* |
| C18 | 0.4850 (5) | 0.1061 (4) | 1.3261 (4) | 0.0318 (11) |
| H18 | 0.519826 | 0.063659 | 1.398103 | 0.038* |
| C19 | 0.3447 (5) | 0.1721 (4) | 1.3075 (4) | 0.0362 (11) |
| H19 | 0.280783 | 0.173765 | 1.365635 | 0.043* |

| | | | | |
|---|---|---|---|---|
| C20 | 0.2994 (5) | 0.2349 (4) | 1.2041 (4) | 0.0316 (11) |
| H20 | 0.203908 | 0.280215 | 1.193139 | 0.038* |
| N12 | 0.3846 (4) | 0.2349 (3) | 1.1175 (3) | 0.0282 (8) |
| O2 | 0.2128 (4) | 0.0355 (4) | 0.4911 (4) | 0.0538 (10) |
| H2A | 0.178 (6) | 0.059 (5) | 0.557 (5) | 0.065* |
| H2B | 0.110 (6) | −0.013 (4) | 0.420 (5) | 0.065* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0320 (4) | 0.0347 (4) | 0.0347 (4) | 0.0178 (3) | 0.0164 (3) | 0.0183 (3) |
| Cl1 | 0.0317 (6) | 0.0400 (7) | 0.0367 (6) | 0.0129 (5) | 0.0136 (5) | 0.0164 (5) |
| O1 | 0.0366 (17) | 0.0391 (18) | 0.0347 (17) | 0.0202 (14) | 0.0200 (14) | 0.0217 (14) |
| C1 | 0.030 (2) | 0.022 (2) | 0.027 (2) | 0.0052 (19) | 0.012 (2) | 0.0094 (19) |
| C2 | 0.027 (2) | 0.034 (3) | 0.032 (2) | 0.0130 (19) | 0.011 (2) | 0.016 (2) |
| O3 | 0.0297 (16) | 0.0351 (17) | 0.0388 (17) | 0.0198 (14) | 0.0135 (13) | 0.0156 (14) |
| C3 | 0.031 (3) | 0.024 (2) | 0.026 (2) | 0.0026 (19) | 0.009 (2) | 0.0098 (19) |
| C4 | 0.025 (2) | 0.032 (3) | 0.030 (2) | 0.0030 (19) | 0.0050 (19) | 0.009 (2) |
| C5 | 0.029 (2) | 0.039 (3) | 0.038 (3) | 0.011 (2) | 0.014 (2) | 0.021 (2) |
| C6 | 0.039 (3) | 0.050 (3) | 0.042 (3) | 0.004 (2) | 0.018 (2) | 0.021 (2) |
| C7 | 0.052 (3) | 0.046 (3) | 0.036 (3) | −0.005 (2) | 0.013 (2) | 0.025 (2) |
| C8 | 0.036 (3) | 0.035 (3) | 0.048 (3) | 0.008 (2) | 0.008 (2) | 0.020 (2) |
| C9 | 0.031 (2) | 0.038 (3) | 0.030 (2) | 0.008 (2) | 0.010 (2) | 0.020 (2) |
| N11 | 0.027 (2) | 0.032 (2) | 0.031 (2) | 0.0111 (16) | 0.0163 (17) | 0.0114 (17) |
| C11 | 0.038 (3) | 0.032 (3) | 0.034 (3) | 0.013 (2) | 0.014 (2) | 0.012 (2) |
| C12 | 0.038 (3) | 0.037 (3) | 0.037 (3) | 0.012 (2) | 0.022 (2) | 0.013 (2) |
| C13 | 0.032 (2) | 0.028 (2) | 0.036 (3) | 0.0114 (19) | 0.015 (2) | 0.013 (2) |
| C14 | 0.034 (2) | 0.028 (2) | 0.027 (2) | 0.0105 (19) | 0.011 (2) | 0.017 (2) |
| C15 | 0.028 (2) | 0.021 (2) | 0.025 (2) | 0.0064 (18) | 0.0106 (19) | 0.0097 (19) |
| C16 | 0.024 (2) | 0.027 (2) | 0.034 (2) | 0.0078 (18) | 0.0102 (19) | 0.013 (2) |
| C17 | 0.034 (2) | 0.024 (2) | 0.034 (3) | 0.0095 (19) | 0.011 (2) | 0.023 (2) |
| C18 | 0.043 (3) | 0.030 (3) | 0.029 (2) | 0.006 (2) | 0.013 (2) | 0.019 (2) |
| C19 | 0.038 (3) | 0.037 (3) | 0.041 (3) | 0.013 (2) | 0.022 (2) | 0.013 (2) |
| C20 | 0.038 (3) | 0.029 (3) | 0.039 (3) | 0.013 (2) | 0.019 (2) | 0.021 (2) |
| N12 | 0.031 (2) | 0.027 (2) | 0.032 (2) | 0.0085 (16) | 0.0155 (17) | 0.0119 (17) |
| O2 | 0.044 (2) | 0.079 (3) | 0.046 (2) | 0.0153 (18) | 0.0187 (17) | 0.028 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.929 (3) | N11—C11 | 1.338 (5) |
| Cu1—O3 | 1.930 (3) | N11—C15 | 1.345 (5) |
| Cu1—N12 | 1.984 (3) | C11—C12 | 1.371 (5) |
| Cu1—N11 | 2.006 (3) | C11—H11 | 0.9500 |
| Cu1—Cl1 | 2.5944 (12) | C12—C13 | 1.387 (5) |
| O1—C1 | 1.270 (4) | C12—H12 | 0.9500 |
| C1—C2 | 1.369 (5) | C13—C14 | 1.372 (5) |
| C1—C1$^{i}$ | 1.537 (7) | C13—H13 | 0.9500 |
| C2—C3 | 1.424 (5) | C14—C15 | 1.383 (5) |

| | | | |
|---|---|---|---|
| C2—H2 | 0.9500 | C14—H14 | 0.9500 |
| O3—C3 | 1.275 (4) | C15—C16 | 1.481 (5) |
| C3—C4 | 1.485 (5) | C16—N12 | 1.371 (5) |
| C4—C5 | 1.390 (5) | C16—C17 | 1.384 (5) |
| C4—C9 | 1.412 (5) | C17—C18 | 1.396 (5) |
| C5—C6 | 1.374 (6) | C17—H17 | 0.9500 |
| C5—H5 | 0.9500 | C18—C19 | 1.393 (5) |
| C6—C7 | 1.378 (6) | C18—H18 | 0.9500 |
| C6—H6 | 0.9500 | C19—C20 | 1.375 (5) |
| C7—C8 | 1.385 (6) | C19—H19 | 0.9500 |
| C7—H7 | 0.9500 | C20—N12 | 1.352 (5) |
| C8—C9 | 1.378 (5) | C20—H20 | 0.9500 |
| C8—H8 | 0.9500 | O2—H2A | 0.82 (5) |
| C9—H9 | 0.9500 | O2—H2B | 0.98 (4) |

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| O1—Cu1—O3 | 93.44 (11) | C4—C9—H9 | 119.4 |
| O1—Cu1—N12 | 89.27 (12) | C11—N11—C15 | 118.8 (3) |
| O3—Cu1—N12 | 167.52 (12) | C11—N11—Cu1 | 125.9 (3) |
| O1—Cu1—N11 | 163.37 (13) | C15—N11—Cu1 | 115.3 (3) |
| O3—Cu1—N11 | 93.59 (12) | N11—C11—C12 | 122.1 (4) |
| N12—Cu1—N11 | 80.78 (13) | N11—C11—H11 | 118.9 |
| O1—Cu1—Cl1 | 95.59 (9) | C12—C11—H11 | 118.9 |
| O3—Cu1—Cl1 | 94.10 (9) | C11—C12—C13 | 119.3 (4) |
| N12—Cu1—Cl1 | 97.76 (10) | C11—C12—H12 | 120.4 |
| N11—Cu1—Cl1 | 98.92 (9) | C13—C12—H12 | 120.4 |
| C1—O1—Cu1 | 122.0 (2) | C14—C13—C12 | 118.9 (4) |
| O1—C1—C2 | 126.3 (4) | C14—C13—H13 | 120.6 |
| O1—C1—C1$^{i}$ | 115.8 (4) | C12—C13—H13 | 120.6 |
| C2—C1—C1$^{i}$ | 117.8 (5) | C13—C14—C15 | 119.1 (4) |
| C1—C2—C3 | 125.1 (4) | C13—C14—H14 | 120.4 |
| C1—C2—H2 | 117.4 | C15—C14—H14 | 120.4 |
| C3—C2—H2 | 117.4 | N11—C15—C14 | 121.9 (4) |
| C3—O3—Cu1 | 123.6 (3) | N11—C15—C16 | 114.7 (3) |
| O3—C3—C2 | 123.4 (4) | C14—C15—C16 | 123.5 (4) |
| O3—C3—C4 | 116.9 (4) | N12—C16—C17 | 121.7 (4) |
| C2—C3—C4 | 119.7 (4) | N12—C16—C15 | 113.3 (3) |
| C5—C4—C9 | 117.5 (4) | C17—C16—C15 | 125.0 (3) |
| C5—C4—C3 | 119.9 (4) | C16—C17—C18 | 119.7 (4) |
| C9—C4—C3 | 122.6 (4) | C16—C17—H17 | 120.2 |
| C6—C5—C4 | 121.2 (4) | C18—C17—H17 | 120.2 |
| C6—C5—H5 | 119.4 | C19—C18—C17 | 118.3 (4) |
| C4—C5—H5 | 119.4 | C19—C18—H18 | 120.8 |
| C5—C6—C7 | 120.5 (4) | C17—C18—H18 | 120.8 |
| C5—C6—H6 | 119.7 | C20—C19—C18 | 119.4 (4) |
| C7—C6—H6 | 119.7 | C20—C19—H19 | 120.3 |
| C6—C7—C8 | 119.9 (4) | C18—C19—H19 | 120.3 |
| C6—C7—H7 | 120.0 | N12—C20—C19 | 122.9 (4) |
| C8—C7—H7 | 120.0 | N12—C20—H20 | 118.5 |

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| C9—C8—C7 | 119.7 (4) | C19—C20—H20 | 118.5 |
| C9—C8—H8 | 120.2 | C20—N12—C16 | 118.0 (4) |
| C7—C8—H8 | 120.2 | C20—N12—Cu1 | 126.2 (3) |
| C8—C9—C4 | 121.2 (4) | C16—N12—Cu1 | 115.9 (3) |
| C8—C9—H9 | 119.4 | H2A—O2—H2B | 96 (4) |
| | | | |
| Cu1—O1—C1—C2 | −16.0 (6) | C11—C12—C13—C14 | −0.4 (6) |
| Cu1—O1—C1—C1$^{i}$ | 165.1 (3) | C12—C13—C14—C15 | 0.1 (6) |
| O1—C1—C2—C3 | −4.0 (7) | C11—N11—C15—C14 | 1.3 (6) |
| C1$^{i}$—C1—C2—C3 | 174.9 (4) | Cu1—N11—C15—C14 | −179.5 (3) |
| Cu1—O3—C3—C2 | 12.9 (5) | C11—N11—C15—C16 | 179.4 (3) |
| Cu1—O3—C3—C4 | −168.5 (2) | Cu1—N11—C15—C16 | −1.4 (4) |
| C1—C2—C3—O3 | 5.8 (6) | C13—C14—C15—N11 | −0.6 (6) |
| C1—C2—C3—C4 | −172.7 (4) | C13—C14—C15—C16 | −178.5 (4) |
| O3—C3—C4—C5 | 15.4 (6) | N11—C15—C16—N12 | 1.4 (5) |
| C2—C3—C4—C5 | −166.0 (4) | C14—C15—C16—N12 | 179.5 (3) |
| O3—C3—C4—C9 | −165.8 (4) | N11—C15—C16—C17 | 179.8 (4) |
| C2—C3—C4—C9 | 12.9 (6) | C14—C15—C16—C17 | −2.1 (6) |
| C9—C4—C5—C6 | −0.7 (6) | N12—C16—C17—C18 | −1.8 (6) |
| C3—C4—C5—C6 | 178.2 (4) | C15—C16—C17—C18 | 179.9 (4) |
| C4—C5—C6—C7 | 1.2 (7) | C16—C17—C18—C19 | 1.8 (6) |
| C5—C6—C7—C8 | −0.4 (7) | C17—C18—C19—C20 | −1.3 (6) |
| C6—C7—C8—C9 | −0.8 (6) | C18—C19—C20—N12 | 0.6 (6) |
| C7—C8—C9—C4 | 1.3 (6) | C19—C20—N12—C16 | −0.4 (6) |
| C5—C4—C9—C8 | −0.6 (6) | C19—C20—N12—Cu1 | 179.9 (3) |
| C3—C4—C9—C8 | −179.4 (4) | C17—C16—N12—C20 | 1.0 (6) |
| C15—N11—C11—C12 | −1.7 (6) | C15—C16—N12—C20 | 179.5 (3) |
| Cu1—N11—C11—C12 | 179.3 (3) | C17—C16—N12—Cu1 | −179.2 (3) |
| N11—C11—C12—C13 | 1.2 (6) | C15—C16—N12—Cu1 | −0.7 (4) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*A*···Cl1 | 0.82 (5) | 2.41 (5) | 3.224 (3) | 171 (5) |
| O2—H2*B*···Cl1$^{ii}$ | 0.98 (4) | 2.33 (5) | 3.307 (4) | 172 (4) |

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