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Bis(μ-3-chlorobenzene-1,2-dicarboxylato-κ^2O^2:O^2)bis[diaqua(5,5′-dimethyl-2,2′-bipyridine-κ^2N,N')copper(II)]

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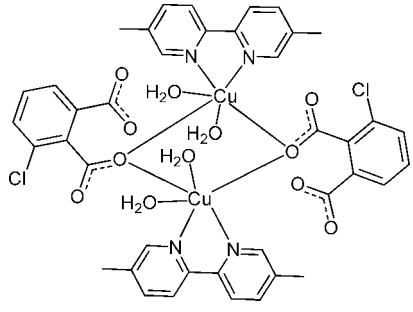
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 12.6.

In the centrosymmetric binuclear title compound, $[Cu_2(C_8H_3ClO_4)_2(C_{12}H_{12}N_2)_2(H_2O)_4]$, the Cu^{II} ion is six-coordinated by two N atoms from a 5,5′-dimethyl-2,2′-bipyridine ligand, two bridging O atoms from two 3-chlorobenzene-1,2-dicarboxylate ligands and two water molecules in a distorted octahedral geometry. The binuclear complex molecules are linked together by intermolecular O—H···O hydrogen bonds into a layer parallel to (100). The layers are connected by C—H···Cl hydrogen bonds. Intramolecular O—H···O hydrogen bonds and π–π interactions [centroid–centroid distance = 3.5958 (16) Å] are also present.

Related literature

For background to polynuclear coordination compounds containing benzenecarboxylate ligands, see: Baca *et al.* (2005); Ma *et al.* (2004); Thirumurugan & Rao (2005); Zang *et al.* (2010). For O—H···O and C—H···Cl hydrogen bonds, see: Desiraju (2004); Song & Iyoda (2009); Wang *et al.* (2011).



Experimental

Crystal data

$[Cu_2(C_8H_3ClO_4)_2(C_{12}H_{12}N_2)_2(H_2O)_4]$
M_r = 964.72
Monoclinic, $P2_1/c$
a = 11.6908 (7) Å
b = 11.8643 (6) Å
c = 17.2869 (13) Å
β = 124.806 (5)°
V = 1968.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 296 K
0.21 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.774, T_{max} = 0.792
7602 measured reflections
3450 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.07
3450 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O3	0.85	1.79	2.622 (3)	164
O1W—H1WB···O4^{i}	0.85	1.82	2.655 (3)	167
O2W—H2WA···O1	0.85	2.17	2.731 (3)	124
O2W—H2WB···O4^{i}	0.85	2.06	2.786 (3)	143
C6—H6···Cl1^{ii}	0.93	2.82	3.609 (4)	144

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

We thank the Science Research Foundation for High-level Talents of Pingdingshan University (No. 2006046) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2462).

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supporting information

Acta Cryst. (2011). E**67**, m1366 [https://doi.org/10.1107/S1600536811035112]

Bis(*μ*-3-chlorobenzene-1,2-dicarboxylato-κ^2O^2:O^2)bis[diaqua(5,5′-dimethyl-2,2′-bipyridine-κ^2N,N')copper(II)]

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S1. Comment

It is common knowledge that the coordination geometry of metal ion and the shape and bonding mode of ligand are generally the primary considerations in metal-mediated self-assembly reactions. Relatively small changes in the bridging ligand can give rise to large variation in the overall structure of the assembly. Recently, some polynuclear coordination compounds containing benzenecarboxylate ligands and O—H···O and C—H···Cl hydrogen bonds (Desiraju, 2004; Song & Iyoda, 2009; Wang *et al.*, 2011) have been reported (Baca *et al.*, 2005; Ma *et al.*, 2004; Thirumurugan & Rao, 2005; Zang *et al.*, 2010). To better understand the influence of benzenecarboxylate ligands and hydrogen-bonding interactions on the resultant structures, we have begun working on the architectures of polynuclear structures from 3-chloro-benzene-1,2-dioic acid. As part of our ongoing investigation, the title compound has been prepared and its structure was determined.

The title compound is a binuclear complex (Fig. 1). The Cu^{II} atom is coordinated by two N atoms from a 5,5′-dimethyl-2,2′-bipyridine ligand, two O atoms from two 3-chlorobenzene-1,2-dicarboxylate ligands and two O atoms from two coordinated water molecules, forming a distorted octahedral geometry. As shown in Fig. 2, each complex molecule is connected to four neighboring molecules through O—H···O hydrogen bonds (Table 1), resulting in a two-dimensional supramolecular structure parallel to (1 0 0). Adjacent layers are associated together by C—H···Cl hydrogen bonds, forming a three-dimensional supramolecular structure (Fig. 3).

S2. Experimental

A mixture of $CuSO_4.5H_2O$ (7.5 mg, 0.03 mmol), 3-chlorobenzene-1,2-dioic acid (6 mg, 0.03 mmol), 5,5′-dimethyl-2,2′-bipyridine (5.5 mg, 0.03 mmol) and NaOH (2.4 mg, 0.06 mmol) in 10 ml of H_2O was sealed in a stainless-steel reactor with a Teflon liner and heated at 393 K for 72 h. A quantity of green single crystals was obtained after the solution was cooled to room temperature at a rate of 10 K h^{-1}.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic) and 0.96 (methyl) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C). H atoms of the water molecules were located from a difference Fourier map and refined with a distance restraint of O—H = 0.85 Å and with U_{iso}(H) = 1.5U_{eq}(O).

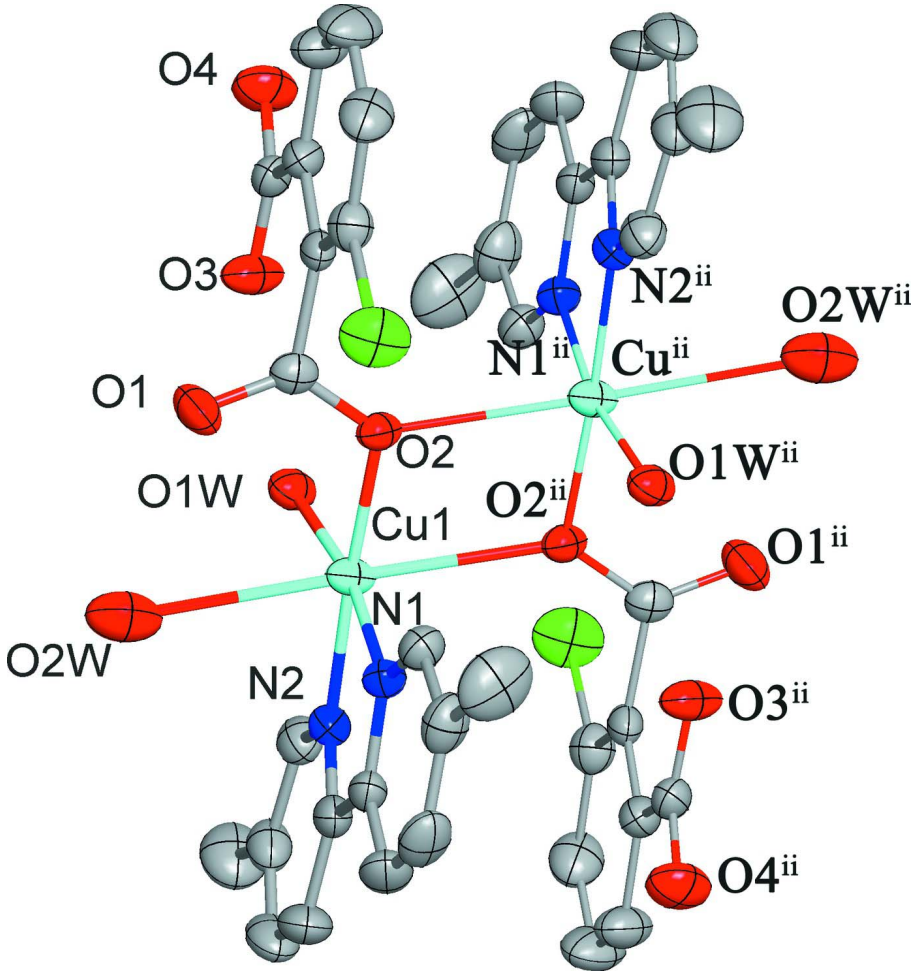

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. [Symmetry code: (i) -x, 2-y, 1-z.]

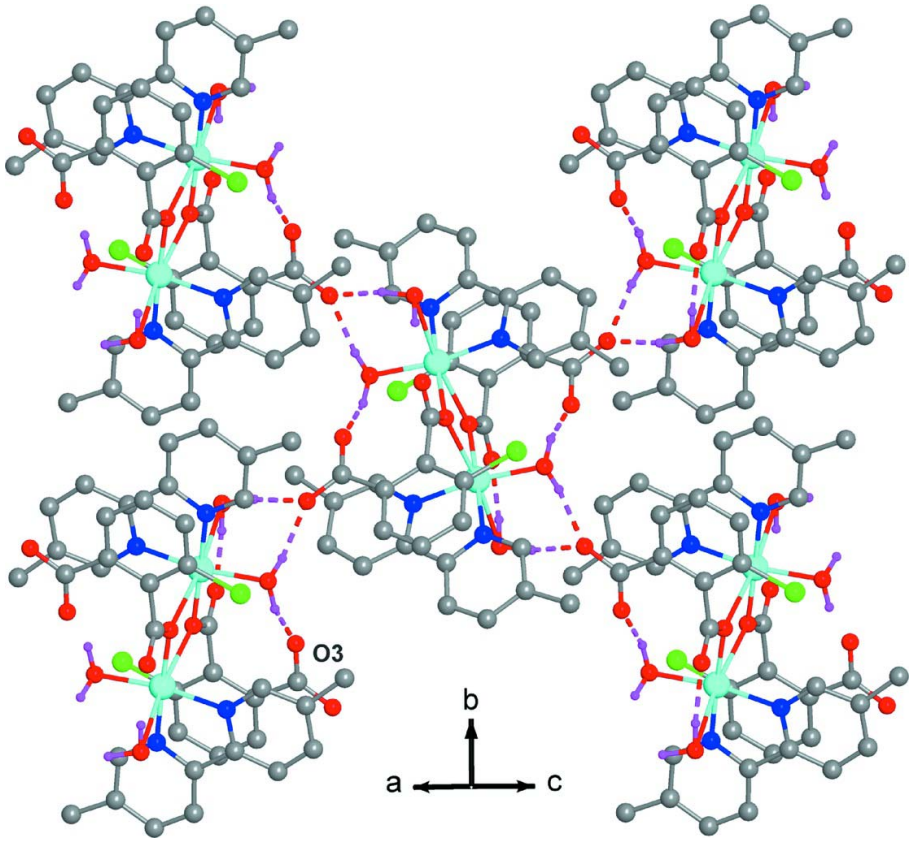

Figure 2

A view of the supramolecular layer in the title compound. Dotted lines represent hydrogen bonds.

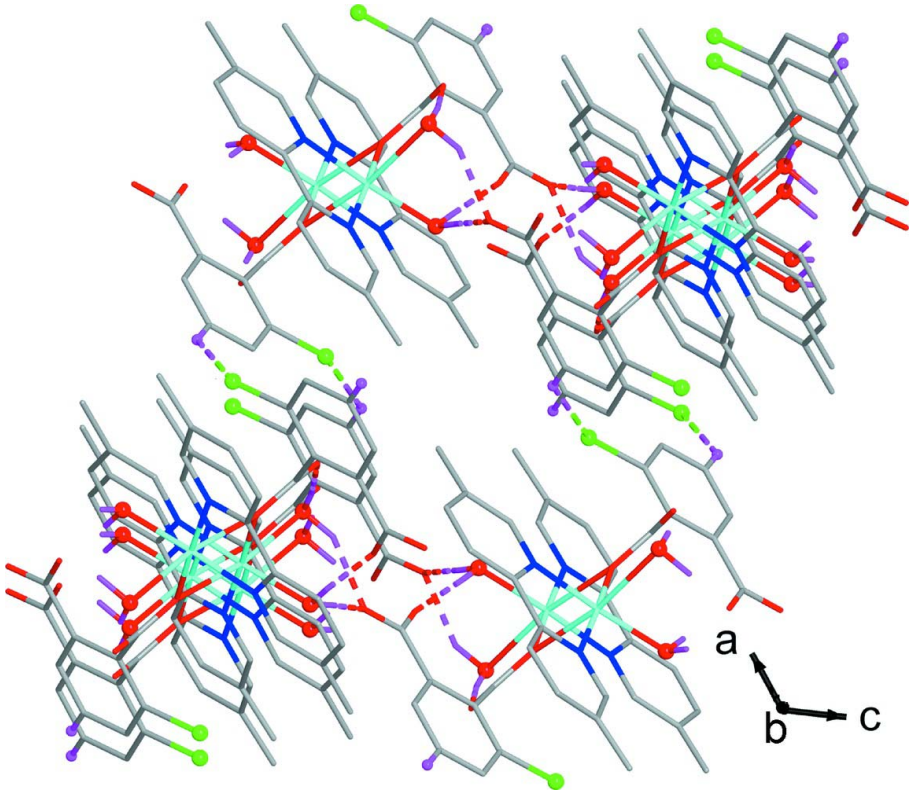

Figure 3

The three-dimensional supramolecular structure in the title compound. Dashed lines indicate hydrogen bonds.

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$c = 17.2869\ (13)$ Å
$\beta = 124.806\ (5)°$
$V = 1968.8\ (2)$ Å^3
$Z = 2$
$F(000) = 988$
$D_x = 1.627$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2332 reflections
$\theta = 3.0–29.3°$
$\mu = 1.29$ mm^{-1}
$T = 296$ K
Block, green
0.21 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.774$, $T_{max} = 0.792$
7602 measured reflections
3450 independent reflections
2845 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$h = -13\rightarrow12$
$k = -13\rightarrow14$
$l = -19\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.07$
3450 reflections
273 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
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.00030 (3)	0.85763 (3)	0.53560 (2)	0.02829 (13)
O1	0.2700 (2)	0.90830 (15)	0.72939 (15)	0.0422 (5)
O2	0.11583 (17)	0.99350 (14)	0.59290 (12)	0.0273 (4)
O3	0.0506 (2)	1.03936 (16)	0.73724 (14)	0.0417 (5)
O4	0.0696 (2)	1.19348 (17)	0.81467 (15)	0.0481 (6)
O1W	−0.08536 (18)	0.88808 (15)	0.60396 (13)	0.0323 (4)
H1WA	−0.0475	0.9459	0.6386	0.048*
H1WB	−0.0733	0.8317	0.6382	0.048*
O2W	0.1570 (2)	0.69797 (18)	0.67213 (17)	0.0595 (7)
H2WA	0.2298	0.7286	0.7187	0.089*
H2WB	0.1093	0.6695	0.6903	0.089*
N1	0.0910 (2)	0.80054 (17)	0.47615 (15)	0.0283 (5)
N2	−0.1213 (2)	0.72318 (17)	0.47124 (15)	0.0291 (5)
C1	0.2153 (3)	0.9926 (2)	0.68096 (18)	0.0275 (6)
C2	0.1059 (3)	1.1301 (2)	0.77408 (19)	0.0294 (6)
C3	0.2744 (3)	1.1063 (2)	0.72625 (18)	0.0262 (6)
C4	0.2292 (3)	1.1679 (2)	0.77316 (19)	0.0313 (7)
C5	0.2972 (3)	1.2677 (2)	0.8182 (2)	0.0442 (8)
H5	0.2670	1.3091	0.8490	0.053*
C6	0.4079 (4)	1.3067 (3)	0.8183 (2)	0.0535 (9)
H6	0.4529	1.3728	0.8501	0.064*
C7	0.4520 (3)	1.2485 (3)	0.7716 (2)	0.0438 (8)
H7	0.5257	1.2751	0.7704	0.053*
C8	0.3848 (3)	1.1490 (2)	0.7262 (2)	0.0332 (7)
C9	0.1929 (3)	0.8511 (2)	0.47533 (19)	0.0329 (7)
H9	0.2267	0.9196	0.5066	0.040*
C10	0.2500 (3)	0.8080 (3)	0.4313 (2)	0.0430 (8)
C11	0.3573 (4)	0.8730 (3)	0.4275 (3)	0.0691 (11)
H11A	0.3784	0.9420	0.4621	0.104*
H11B	0.3214	0.8898	0.3631	0.104*
H11C	0.4405	0.8287	0.4548	0.104*
C12	0.2011 (3)	0.7028 (3)	0.3883 (2)	0.0457 (8)
H12	0.2390	0.6687	0.3593	0.055*
C13	0.0978 (3)	0.6501 (2)	0.3887 (2)	0.0432 (8)

H13	0.0651	0.5803	0.3599	0.052*
C14	0.0421 (3)	0.7003 (2)	0.43179 (18)	0.0290 (6)
C15	−0.0748 (3)	0.6550 (2)	0.43229 (19)	0.0317 (7)
C16	−0.1362 (3)	0.5512 (2)	0.3958 (2)	0.0435 (8)
H16	−0.1047	0.5051	0.3682	0.052*
C17	−0.2437 (3)	0.5169 (2)	0.4008 (2)	0.0482 (9)
H17	−0.2842	0.4467	0.3772	0.058*
C18	−0.2924 (3)	0.5854 (2)	0.4403 (2)	0.0398 (7)
C19	−0.4090 (3)	0.5521 (3)	0.4481 (3)	0.0620 (10)
H19A	−0.4961	0.5765	0.3929	0.093*
H19B	−0.3959	0.5867	0.5028	0.093*
H19C	−0.4099	0.4716	0.4536	0.093*
C20	−0.2279 (3)	0.6894 (2)	0.4739 (2)	0.0353 (7)
H20	−0.2605	0.7379	0.4995	0.042*
Cl1	0.44008 (8)	1.07793 (7)	0.66549 (6)	0.0534 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0343 (2)	0.0238 (2)	0.0340 (2)	−0.00589 (14)	0.02376 (18)	−0.00736 (15)
O1	0.0441 (12)	0.0252 (10)	0.0467 (13)	0.0041 (10)	0.0196 (10)	0.0063 (10)
O2	0.0310 (10)	0.0261 (9)	0.0260 (10)	−0.0061 (8)	0.0170 (9)	−0.0060 (9)
O3	0.0569 (13)	0.0368 (11)	0.0489 (13)	−0.0175 (10)	0.0405 (11)	−0.0177 (10)
O4	0.0625 (14)	0.0416 (12)	0.0574 (15)	0.0008 (11)	0.0444 (13)	−0.0117 (11)
O1W	0.0441 (11)	0.0252 (9)	0.0366 (11)	−0.0045 (9)	0.0284 (10)	−0.0031 (9)
O2W	0.0635 (15)	0.0554 (14)	0.0714 (17)	−0.0126 (12)	0.0455 (14)	−0.0206 (13)
N1	0.0357 (13)	0.0248 (12)	0.0271 (12)	0.0010 (10)	0.0194 (11)	−0.0024 (10)
N2	0.0336 (13)	0.0242 (11)	0.0271 (12)	−0.0014 (10)	0.0159 (11)	0.0003 (10)
C1	0.0281 (14)	0.0294 (14)	0.0321 (16)	−0.0001 (12)	0.0213 (13)	−0.0032 (13)
C2	0.0386 (16)	0.0265 (14)	0.0246 (14)	0.0025 (13)	0.0190 (13)	0.0014 (12)
C3	0.0278 (14)	0.0233 (13)	0.0202 (13)	−0.0004 (12)	0.0094 (12)	0.0033 (12)
C4	0.0399 (16)	0.0258 (13)	0.0260 (15)	−0.0024 (13)	0.0175 (13)	−0.0008 (13)
C5	0.062 (2)	0.0355 (16)	0.0428 (19)	−0.0137 (16)	0.0344 (17)	−0.0129 (15)
C6	0.073 (2)	0.0365 (17)	0.056 (2)	−0.0237 (17)	0.040 (2)	−0.0156 (17)
C7	0.0390 (16)	0.0455 (18)	0.0418 (19)	−0.0152 (15)	0.0200 (15)	−0.0018 (16)
C8	0.0296 (15)	0.0365 (15)	0.0323 (16)	0.0012 (13)	0.0170 (13)	0.0029 (14)
C9	0.0379 (16)	0.0341 (15)	0.0286 (15)	0.0016 (13)	0.0200 (14)	−0.0002 (13)
C10	0.0429 (18)	0.057 (2)	0.0355 (17)	0.0078 (16)	0.0265 (15)	0.0077 (16)
C11	0.066 (2)	0.099 (3)	0.069 (3)	−0.013 (2)	0.055 (2)	−0.007 (2)
C12	0.056 (2)	0.056 (2)	0.0368 (18)	0.0155 (17)	0.0341 (17)	0.0012 (16)
C13	0.061 (2)	0.0343 (16)	0.0388 (18)	0.0077 (15)	0.0313 (17)	−0.0042 (15)
C14	0.0376 (16)	0.0250 (14)	0.0227 (14)	0.0053 (12)	0.0162 (13)	0.0025 (12)
C15	0.0393 (17)	0.0251 (14)	0.0233 (14)	0.0022 (13)	0.0134 (13)	0.0021 (12)
C16	0.057 (2)	0.0276 (15)	0.0389 (18)	−0.0044 (15)	0.0233 (16)	−0.0087 (14)
C17	0.050 (2)	0.0288 (15)	0.0441 (19)	−0.0129 (15)	0.0141 (16)	−0.0029 (15)
C18	0.0358 (16)	0.0363 (16)	0.0326 (16)	−0.0078 (14)	0.0109 (14)	0.0044 (15)
C19	0.050 (2)	0.058 (2)	0.067 (2)	−0.0219 (18)	0.0273 (19)	−0.002 (2)
C20	0.0314 (15)	0.0360 (15)	0.0314 (16)	−0.0018 (13)	0.0138 (13)	0.0011 (14)

Cl1	0.0504 (5)	0.0573 (5)	0.0724 (6)	−0.0032 (4)	0.0468 (5)	−0.0078 (5)

Geometric parameters (Å, º)

Cu1—O2	1.9689 (16)	C7—C8	1.387 (4)
Cu1—O2^{i}	2.5406 (17)	C7—H7	0.9300
Cu1—N1	1.971 (2)	C8—Cl1	1.733 (3)
Cu1—N2	2.000 (2)	C9—C10	1.366 (4)
Cu1—O1W	1.9700 (19)	C9—H9	0.9300
Cu1—O2W	2.753 (2)	C10—C12	1.397 (4)
O1—C1	1.224 (3)	C10—C11	1.506 (4)
O2—C1	1.284 (3)	C11—H11A	0.9600
O3—C2	1.230 (3)	C11—H11B	0.9600
O4—C2	1.256 (3)	C11—H11C	0.9600
O1W—H1WA	0.8500	C12—C13	1.363 (4)
O1W—H1WB	0.8500	C12—H12	0.9300
O2W—H2WA	0.8500	C13—C14	1.373 (4)
O2W—H2WB	0.8500	C13—H13	0.9300
N1—C9	1.341 (3)	C14—C15	1.474 (4)
N1—C14	1.352 (3)	C15—C16	1.382 (4)
N2—C20	1.334 (3)	C16—C17	1.370 (4)
N2—C15	1.350 (4)	C16—H16	0.9300
C1—C3	1.514 (4)	C17—C18	1.376 (4)
C2—C4	1.518 (4)	C17—H17	0.9300
C3—C8	1.387 (4)	C18—C20	1.389 (4)
C3—C4	1.400 (4)	C18—C19	1.498 (4)
C4—C5	1.390 (4)	C19—H19A	0.9600
C5—C6	1.373 (4)	C19—H19B	0.9600
C5—H5	0.9300	C19—H19C	0.9600
C6—C7	1.367 (5)	C20—H20	0.9300
C6—H6	0.9300		
O2—Cu1—O1W	89.18 (7)	C6—C7—H7	120.6
O2—Cu1—N1	97.18 (8)	C8—C7—H7	120.6
O1W—Cu1—N1	170.06 (8)	C7—C8—C3	122.5 (3)
O2—Cu1—N2	177.20 (8)	C7—C8—Cl1	118.1 (2)
O1W—Cu1—N2	92.09 (9)	C3—C8—Cl1	119.4 (2)
N1—Cu1—N2	81.90 (9)	N1—C9—C10	123.9 (3)
O2—Cu1—O2W	101.68 (7)	N1—C9—H9	118.1
O1W—Cu1—O2W	85.94 (7)	C10—C9—H9	118.1
N1—Cu1—O2W	85.29 (8)	C9—C10—C12	116.7 (3)
N2—Cu1—O2W	80.91 (8)	C9—C10—C11	121.1 (3)
O1W—Cu1—O2^{i}	101.31 (7)	C12—C10—C11	122.1 (3)
N1—Cu1—O2^{i}	87.77 (8)	C10—C11—H11A	109.5
O2—Cu1—O2^{i}	75.02 (7)	C10—C11—H11B	109.5
O2W—Cu1—O2^{i}	171.88 (8)	H11A—C11—H11B	109.5
N2—Cu1—O2^{i}	102.28 (7)	C10—C11—H11C	109.5
C1—O2—Cu1	119.12 (17)	H11A—C11—H11C	109.5

Cu1—O1W—H1WA	109.4	H11B—C11—H11C	109.5
Cu1—O1W—H1WB	109.5	C13—C12—C10	120.1 (3)
H1WA—O1W—H1WB	109.5	C13—C12—H12	120.0
Cu1—O2W—H2WA	109.5	C10—C12—H12	120.0
Cu1—O2W—H2WB	109.5	C12—C13—C14	120.0 (3)
H2WA—O2W—H2WB	109.5	C12—C13—H13	120.0
C9—N1—C14	118.6 (2)	C14—C13—H13	120.0
C9—N1—Cu1	126.69 (18)	N1—C14—C13	120.7 (3)
C14—N1—Cu1	114.75 (18)	N1—C14—C15	114.3 (2)
C20—N2—C15	119.2 (2)	C13—C14—C15	125.0 (3)
C20—N2—Cu1	127.0 (2)	N2—C15—C16	120.6 (3)
C15—N2—Cu1	113.24 (18)	N2—C15—C14	115.1 (2)
O1—C1—O2	125.7 (2)	C16—C15—C14	124.3 (3)
O1—C1—C3	117.9 (2)	C17—C16—C15	119.5 (3)
O2—C1—C3	116.3 (2)	C17—C16—H16	120.3
O3—C2—O4	124.6 (3)	C15—C16—H16	120.3
O3—C2—C4	118.4 (2)	C16—C17—C18	120.7 (3)
O4—C2—C4	117.0 (2)	C16—C17—H17	119.7
C8—C3—C4	118.0 (2)	C18—C17—H17	119.7
C8—C3—C1	118.4 (2)	C17—C18—C20	116.9 (3)
C4—C3—C1	123.6 (2)	C17—C18—C19	123.0 (3)
C5—C4—C3	119.0 (3)	C20—C18—C19	120.1 (3)
C5—C4—C2	119.3 (3)	C18—C19—H19A	109.5
C3—C4—C2	121.7 (2)	C18—C19—H19B	109.5
C6—C5—C4	121.7 (3)	H19A—C19—H19B	109.5
C6—C5—H5	119.2	C18—C19—H19C	109.5
C4—C5—H5	119.2	H19A—C19—H19C	109.5
C7—C6—C5	120.1 (3)	H19B—C19—H19C	109.5
C7—C6—H6	120.0	N2—C20—C18	123.1 (3)
C5—C6—H6	120.0	N2—C20—H20	118.4
C6—C7—C8	118.8 (3)	C18—C20—H20	118.4

O1W—Cu1—O2—C1	71.57 (19)	C4—C3—C8—C7	0.9 (4)
N1—Cu1—O2—C1	−100.76 (19)	C1—C3—C8—C7	−175.4 (3)
O2W—Cu1—O2—C1	−14.12 (19)	C4—C3—C8—Cl1	−177.8 (2)
O2—Cu1—N1—C9	−3.7 (2)	C1—C3—C8—Cl1	5.9 (3)
N2—Cu1—N1—C9	173.6 (2)	C14—N1—C9—C10	0.7 (4)
O2W—Cu1—N1—C9	−104.9 (2)	Cu1—N1—C9—C10	−178.8 (2)
O2—Cu1—N1—C14	176.77 (18)	N1—C9—C10—C12	−2.5 (4)
N2—Cu1—N1—C14	−5.90 (18)	N1—C9—C10—C11	175.7 (3)
O2W—Cu1—N1—C14	75.57 (18)	C9—C10—C12—C13	2.2 (5)
O1W—Cu1—N2—C20	7.1 (2)	C11—C10—C12—C13	−176.0 (3)
N1—Cu1—N2—C20	179.1 (2)	C10—C12—C13—C14	−0.2 (5)
O2W—Cu1—N2—C20	92.6 (2)	C9—N1—C14—C13	1.5 (4)
O1W—Cu1—N2—C15	−163.93 (18)	Cu1—N1—C14—C13	−178.9 (2)
N1—Cu1—N2—C15	8.11 (18)	C9—N1—C14—C15	−176.8 (2)
O2W—Cu1—N2—C15	−78.38 (18)	Cu1—N1—C14—C15	2.8 (3)
Cu1—O2—C1—O1	19.6 (4)	C12—C13—C14—N1	−1.7 (4)

Cu1—O2—C1—C3	−164.18 (17)	C12—C13—C14—C15	176.3 (3)
O1—C1—C3—C8	86.6 (3)	C20—N2—C15—C16	−0.2 (4)
O2—C1—C3—C8	−89.9 (3)	Cu1—N2—C15—C16	171.6 (2)
O1—C1—C3—C4	−89.5 (3)	C20—N2—C15—C14	179.4 (2)
O2—C1—C3—C4	94.0 (3)	Cu1—N2—C15—C14	−8.8 (3)
C8—C3—C4—C5	−0.7 (4)	N1—C14—C15—N2	4.1 (3)
C1—C3—C4—C5	175.4 (3)	C13—C14—C15—N2	−174.0 (3)
C8—C3—C4—C2	177.8 (2)	N1—C14—C15—C16	−176.3 (3)
C1—C3—C4—C2	−6.1 (4)	C13—C14—C15—C16	5.5 (4)
O3—C2—C4—C5	−177.1 (3)	N2—C15—C16—C17	−1.0 (4)
O4—C2—C4—C5	1.4 (4)	C14—C15—C16—C17	179.4 (3)
O3—C2—C4—C3	4.5 (4)	C15—C16—C17—C18	1.0 (4)
O4—C2—C4—C3	−177.1 (3)	C16—C17—C18—C20	0.2 (4)
C3—C4—C5—C6	−0.5 (5)	C16—C17—C18—C19	−179.7 (3)
C2—C4—C5—C6	−179.0 (3)	C15—N2—C20—C18	1.5 (4)
C4—C5—C6—C7	1.4 (5)	Cu1—N2—C20—C18	−169.0 (2)
C5—C6—C7—C8	−1.2 (5)	C17—C18—C20—N2	−1.5 (4)
C6—C7—C8—C3	0.0 (5)	C19—C18—C20—N2	178.3 (3)
C6—C7—C8—Cl1	178.7 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3	0.85	1.79	2.622 (3)	164
O1*W*—H1*WB*···O4^{ii}	0.85	1.82	2.655 (3)	167
O2*W*—H2*WA*···O1	0.85	2.17	2.731 (3)	124
O2*W*—H2*WB*···O4^{ii}	0.85	2.06	2.786 (3)	143
C6—H6···Cl1^{iii}	0.93	2.82	3.609 (4)	144

Symmetry codes: (ii) −*x*, *y*−1/2, −*z*+3/2; (iii) −*x*+1, *y*+1/2, −*z*+3/2.