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Bis(μ-3-nitrophthalato-κ²O¹:O²)-bis[aqua(2,2′-bipyridine-κ²N,N′)-copper(II)] dihydrate

Yin-Feng Han,[a] Chen Cheng[b] and Seik Weng Ng[c]*

[a]Department of Chemistry and Chemical Engineering, Baoji University of Arts and Science, Baoji 721013, People's Republic of China, [b]Department of Biotechnology, Wulanchabu Vocational College, Wulanchabu 012000, Inner Mongolia, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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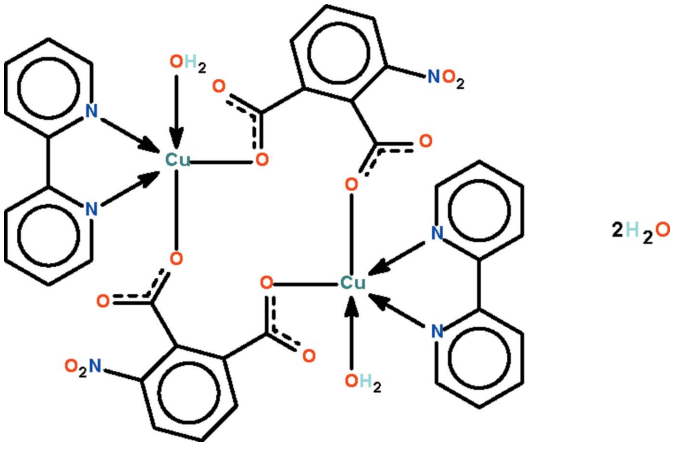
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.088; data-to-parameter ratio = 10.9.

Two 3-nitrophthalate dianions bridge two water-coordinated 2,2′-bipyridine-chelated Cu^{II} atoms about a center of inversion to generate the title dinuclear compound, $[Cu_2(C_8H_3NO_6)_2(C_{10}H_8N_2)_2(H_2O)_2]\cdot 2H_2O$. The geometry of the Cu^{II} atom is a distorted square pyramid. Adjacent molecules are linked through the coordinated and solvent water molecules to form a linear ribbon running along the a axis of the monoclinic unit cell.

Related literature

For the isostructural zinc analog, see: Song *et al.* (2007).



Experimental

Crystal data

$[Cu_2(C_8H_3NO_6)_2(C_{10}H_8N_2)_2(H_2O)_2]\cdot 2H_2O$
M_r = 929.74
Triclinic, $P\overline{1}$
a = 7.534 (2) Å
b = 10.467 (3) Å
c = 12.044 (3) Å
α = 87.835 (2)°
β = 74.911 (3)°
γ = 77.437 (3)°
V = 894.9 (4) Å³
Z = 1
Mo $K\alpha$ radiation
μ = 1.28 mm⁻¹
T = 295 K
0.45 × 0.45 × 0.40 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.591, T_{max} = 0.629
4675 measured reflections
3092 independent reflections
2732 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.01
3092 reflections
284 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å⁻³
$\Delta\rho_{min}$ = −0.55 e Å⁻³

Table 1
Selected bond lengths (Å).

Cu1—O1	1.967 (2)	Cu1—N2	2.029 (2)
Cu1—O3^{i}	2.172 (2)	Cu1—N3	2.013 (2)
Cu1—O1w	1.994 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2w	0.83 (3)	1.85 (1)	2.660 (3)	166 (3)
O1w—H12···O4^{ii}	0.83 (3)	1.90 (1)	2.718 (3)	168 (3)
O2w—H21···O4	0.84 (3)	2.04 (2)	2.830 (3)	158 (3)
O2w—H22···O1^{i}	0.84 (3)	2.25 (2)	2.985 (3)	146 (3)
O2w—H22···O3^{i}	0.84 (3)	2.35 (3)	2.977 (3)	132 (3)

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5061).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, Y.-S., Yan, B. & Chen, Z.-X. (2007). *Appl. Organomet. Chem.* **21**, 150–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2010). E**66**, m1484 [https://doi.org/10.1107/S1600536810043229]

Bis(*μ*-3-nitrophthalato-κ^2O^1:O^2)bis[aqua(2,2′-bipyridine-κ^2N,N')copper(II)] dihydrate

Yin-Feng Han, Chen Cheng and Seik Weng Ng

S1. Comment

Dinuclear $Zn_2(H_2O)_2(C_{10}H_8N_2)_2(C_8H_3NO_6)_2\cdot 2H_2O$ is reported to exhibit intense fluorescence. In its crystal structure, the 3-nitrophthalate dianion bridges two water-coordinated, 2,2′-bipyridine-chelated zinc atoms about a center-of-inversion; the geometry of the zinc atom is a square pyramid (Song *et al.*, 2007). The present copper analog (Scheme I, Fig. 1) is isostructural, the two compounds crystallizing with matching cell dimensions. Adjacent molecules are connected to the lattice water molecule by hydrogen bonds to form a linear ribbon running along the *a*-axis of the monoclinic unit cell (Fig. 2).

S2. Experimental

3-Nitrophthalic acid (0.105 g), 2,2′-bipyridine (0.078 g), copper chloride dihydrate (0.085 g) and water (2 ml) were heated at 393 K in a 25 ml, Teflon-lined, stainless-steel Parr bomb for 3 days. Blue crystal were isolated. CH&N elemental analysis. Found: C 46.32, H 3.17, N 9.11%. Calc.: C 46.51, H 3.25, N 9.04%.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and H···H 1.37±0.01 Å; their temperature factors were refined.

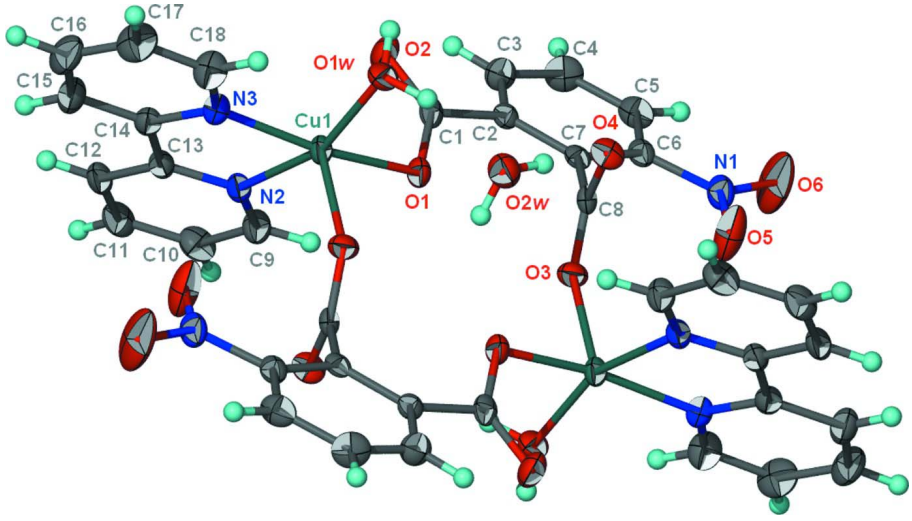

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of dinuclear $Cu_2(H_2O)_2(C_{10}H_8N_2)_2(C_8H_3NO_6)_2{\cdot}2H_2O$ at the 50% probability evel; hydrogen atoms are shown as spheres of arbitrary radius.

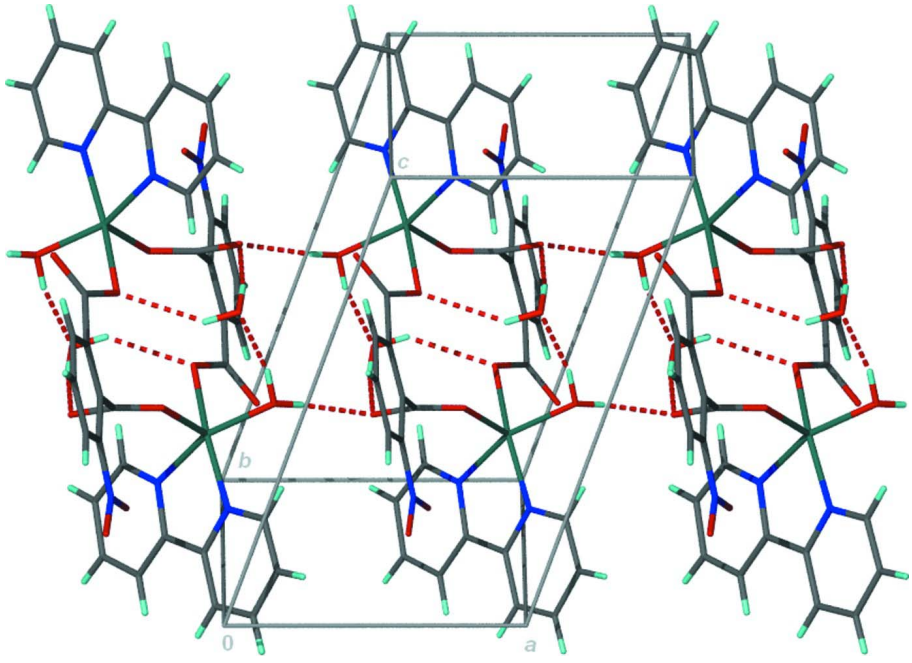

Figure 2

Hydrogen-bonded chain.

Bis(*μ*-3-nitrophthalato-κ^2O^1:O^2)bis[aqua(2,2′- bipyridine-κ^2N,N')copper(II)] dihydrate

Crystal data

$[Cu_2(C_8H_3NO_6)_2(C_{10}H_8N_2)_2(H_2O)_2]{\cdot}2H_2O$
M_r = 929.74
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.534 (2) Å
b = 10.467 (3) Å
c = 12.044 (3) Å
α = 87.835 (2)°
β = 74.911 (3)°
γ = 77.437 (3)°

V = 894.9 (4) Å^3
Z = 1
F(000) = 474
D_x = 1.725 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3039 reflections
θ = 2.6–28.1°
μ = 1.28 mm^{-1}
T = 295 K
Block, blue
0.45 × 0.45 × 0.40 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.591, T_{max} = 0.629
4675 measured reflections
3092 independent reflections
2732 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −6→8
k = −11→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.01
3092 reflections
284 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.6587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.050 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.21328 (4)	0.56513 (3)	0.71332 (2)	0.02412 (15)
N1	0.4799 (3)	0.0616 (2)	0.2658 (2)	0.0343 (6)
N2	0.2998 (3)	0.4783 (2)	0.84926 (18)	0.0257 (5)
N3	0.0759 (3)	0.7029 (2)	0.83612 (19)	0.0281 (5)
O1	0.3115 (3)	0.41035 (18)	0.61015 (15)	0.0280 (4)
O2	0.0466 (3)	0.3577 (2)	0.71082 (17)	0.0409 (5)
O3	0.5866 (2)	0.32313 (18)	0.38170 (15)	0.0288 (4)
O4	0.3075 (3)	0.39837 (18)	0.34247 (16)	0.0305 (4)
O5	0.5574 (4)	0.1439 (2)	0.2160 (2)	0.0633 (8)
O6	0.4884 (5)	−0.0410 (3)	0.2191 (2)	0.0874 (11)
O1W	0.0433 (3)	0.6507 (2)	0.61730 (16)	0.0332 (5)
H11	0.105 (4)	0.646 (3)	0.5489 (12)	0.050*
H12	−0.056 (3)	0.625 (3)	0.626 (2)	0.050*
O2W	0.2753 (3)	0.6602 (2)	0.41019 (18)	0.0385 (5)
H21	0.279 (4)	0.593 (2)	0.374 (3)	0.058*
H22	0.372 (3)	0.650 (3)	0.435 (3)	0.058*
C1	0.1932 (4)	0.3366 (3)	0.6318 (2)	0.0256 (6)
C2	0.2383 (4)	0.2132 (2)	0.5588 (2)	0.0230 (5)

C3	0.1636 (4)	0.1084 (3)	0.6101 (2)	0.0333 (7)
H3	0.0890	0.1179	0.6854	0.040*
C4	0.1973 (4)	−0.0096 (3)	0.5522 (3)	0.0389 (7)
H4	0.1505	−0.0795	0.5892	0.047*
C5	0.3010 (4)	−0.0224 (3)	0.4391 (3)	0.0350 (7)
H5	0.3223	−0.1002	0.3981	0.042*
C6	0.3725 (4)	0.0823 (3)	0.3879 (2)	0.0257 (6)
C7	0.3471 (3)	0.2024 (2)	0.4442 (2)	0.0210 (5)
C8	0.4222 (4)	0.3186 (2)	0.3836 (2)	0.0213 (5)
C9	0.4136 (4)	0.3603 (3)	0.8485 (2)	0.0330 (6)
H9	0.4684	0.3147	0.7789	0.040*
C10	0.4522 (4)	0.3043 (3)	0.9478 (3)	0.0379 (7)
H10	0.5333	0.2229	0.9445	0.045*
C11	0.3696 (4)	0.3698 (3)	1.0513 (3)	0.0383 (7)
H11A	0.3934	0.3332	1.1189	0.046*
C12	0.2507 (4)	0.4911 (3)	1.0534 (2)	0.0340 (7)
H12A	0.1921	0.5369	1.1225	0.041*
C13	0.2199 (4)	0.5435 (3)	0.9505 (2)	0.0266 (6)
C14	0.0971 (4)	0.6732 (3)	0.9424 (2)	0.0281 (6)
C15	0.0074 (4)	0.7584 (3)	1.0353 (3)	0.0395 (7)
H15	0.0244	0.7368	1.1080	0.047*
C16	−0.1067 (5)	0.8752 (3)	1.0185 (3)	0.0474 (8)
H16	−0.1691	0.9332	1.0799	0.057*
C17	−0.1276 (5)	0.9055 (3)	0.9093 (3)	0.0483 (8)
H17	−0.2030	0.9845	0.8961	0.058*
C18	−0.0351 (5)	0.8171 (3)	0.8207 (3)	0.0396 (7)
H18	−0.0501	0.8374	0.7474	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0282 (2)	0.0265 (2)	0.01756 (19)	−0.00328 (14)	−0.00774 (13)	−0.00078 (12)
N1	0.0379 (14)	0.0317 (14)	0.0318 (13)	−0.0003 (11)	−0.0108 (11)	−0.0096 (11)
N2	0.0292 (12)	0.0285 (12)	0.0210 (11)	−0.0074 (10)	−0.0082 (9)	−0.0014 (9)
N3	0.0317 (13)	0.0270 (12)	0.0242 (11)	−0.0058 (10)	−0.0051 (10)	−0.0004 (9)
O1	0.0316 (10)	0.0304 (10)	0.0225 (9)	−0.0080 (8)	−0.0057 (8)	−0.0061 (8)
O2	0.0400 (12)	0.0493 (13)	0.0274 (11)	−0.0112 (10)	0.0044 (9)	−0.0098 (9)
O3	0.0236 (10)	0.0363 (11)	0.0288 (10)	−0.0104 (8)	−0.0080 (8)	0.0044 (8)
O4	0.0328 (10)	0.0280 (10)	0.0334 (10)	−0.0040 (8)	−0.0167 (9)	0.0093 (8)
O5	0.101 (2)	0.0467 (15)	0.0320 (12)	−0.0231 (15)	0.0086 (13)	−0.0070 (11)
O6	0.125 (3)	0.0627 (18)	0.0617 (18)	−0.0406 (19)	0.0202 (18)	−0.0405 (15)
O1W	0.0281 (11)	0.0455 (12)	0.0278 (10)	−0.0052 (9)	−0.0125 (9)	0.0023 (9)
O2W	0.0421 (12)	0.0405 (12)	0.0355 (12)	−0.0119 (10)	−0.0121 (10)	−0.0007 (9)
C1	0.0316 (15)	0.0300 (14)	0.0164 (12)	−0.0039 (12)	−0.0108 (11)	0.0031 (10)
C2	0.0227 (13)	0.0254 (13)	0.0219 (13)	−0.0026 (11)	−0.0097 (11)	0.0020 (10)
C3	0.0349 (16)	0.0368 (16)	0.0281 (14)	−0.0098 (13)	−0.0073 (12)	0.0056 (12)
C4	0.0441 (18)	0.0285 (16)	0.0461 (18)	−0.0150 (14)	−0.0102 (15)	0.0105 (13)
C5	0.0362 (16)	0.0225 (14)	0.0489 (18)	−0.0047 (12)	−0.0167 (14)	−0.0022 (13)

C6	0.0237 (13)	0.0263 (14)	0.0273 (14)	0.0000 (11)	−0.0107 (11)	−0.0033 (11)
C7	0.0195 (12)	0.0221 (13)	0.0234 (13)	−0.0014 (10)	−0.0116 (10)	0.0015 (10)
C8	0.0264 (14)	0.0238 (13)	0.0145 (11)	−0.0053 (11)	−0.0062 (10)	−0.0023 (10)
C9	0.0373 (16)	0.0332 (16)	0.0279 (14)	−0.0022 (13)	−0.0114 (12)	−0.0013 (12)
C10	0.0413 (17)	0.0339 (16)	0.0432 (17)	−0.0056 (13)	−0.0223 (14)	0.0079 (13)
C11	0.0442 (18)	0.0487 (19)	0.0295 (15)	−0.0182 (15)	−0.0178 (14)	0.0138 (13)
C12	0.0375 (16)	0.0489 (18)	0.0206 (13)	−0.0177 (14)	−0.0094 (12)	0.0010 (12)
C13	0.0285 (14)	0.0326 (15)	0.0217 (13)	−0.0120 (12)	−0.0072 (11)	−0.0002 (11)
C14	0.0280 (14)	0.0323 (15)	0.0252 (14)	−0.0121 (12)	−0.0041 (11)	−0.0018 (11)
C15	0.0438 (18)	0.0445 (18)	0.0281 (15)	−0.0139 (15)	−0.0007 (13)	−0.0085 (13)
C16	0.049 (2)	0.0407 (19)	0.0447 (19)	−0.0076 (16)	0.0027 (16)	−0.0164 (15)
C17	0.048 (2)	0.0313 (17)	0.058 (2)	−0.0008 (15)	−0.0065 (17)	−0.0074 (15)
C18	0.0457 (18)	0.0313 (16)	0.0382 (17)	−0.0026 (14)	−0.0096 (14)	0.0018 (13)

Geometric parameters (Å, º)

Cu1—O1	1.967 (2)	C3—H3	0.9300
Cu1—O3^{i}	2.172 (2)	C4—C5	1.378 (4)
Cu1—O1w	1.994 (2)	C4—H4	0.9300
Cu1—N2	2.029 (2)	C5—C6	1.380 (4)
Cu1—N3	2.013 (2)	C5—H5	0.9300
N1—O5	1.199 (3)	C6—C7	1.403 (4)
N1—O6	1.213 (3)	C7—C8	1.533 (3)
N1—C6	1.480 (4)	C9—C10	1.383 (4)
N2—C13	1.348 (3)	C9—H9	0.9300
N2—C9	1.340 (4)	C10—C11	1.373 (4)
N3—C18	1.339 (4)	C10—H10	0.9300
N3—C14	1.347 (4)	C11—C12	1.382 (4)
O1—C1	1.274 (3)	C11—H11A	0.9300
O2—C1	1.240 (3)	C12—C13	1.390 (4)
O3—C8	1.244 (3)	C12—H12A	0.9300
O3—Cu1^{i}	2.1722 (18)	C13—C14	1.483 (4)
O4—C8	1.252 (3)	C14—C15	1.387 (4)
O1W—H11	0.83 (3)	C15—C16	1.374 (5)
O1W—H12	0.83 (3)	C15—H15	0.9300
O2W—H21	0.84 (3)	C16—C17	1.381 (5)
O2W—H22	0.84 (3)	C16—H16	0.9300
C1—C2	1.515 (4)	C17—C18	1.374 (4)
C2—C3	1.393 (4)	C17—H17	0.9300
C2—C7	1.404 (4)	C18—H18	0.9300
C3—C4	1.382 (4)		

O1—Cu1—O1W	92.15 (8)	C5—C6—C7	124.0 (3)
O1—Cu1—N3	168.62 (8)	C5—C6—N1	115.6 (2)
O1W—Cu1—N3	88.44 (9)	C7—C6—N1	120.5 (2)
O1—Cu1—N2	95.88 (8)	C2—C7—C6	116.0 (2)
O1W—Cu1—N2	160.36 (9)	C2—C7—C8	121.2 (2)
N3—Cu1—N2	80.22 (9)	C6—C7—C8	122.7 (2)

O1—Cu1—O3^{i}	95.27 (8)	O3—C8—O4	128.0 (2)
O1W—Cu1—O3^{i}	86.74 (8)	O3—C8—C7	117.1 (2)
N3—Cu1—O3^{i}	96.11 (8)	O4—C8—C7	114.9 (2)
N2—Cu1—O3^{i}	110.24 (8)	N2—C9—C10	122.1 (3)
O5—N1—O6	121.7 (3)	N2—C9—H9	119.0
O5—N1—C6	120.4 (2)	C10—C9—H9	119.0
O6—N1—C6	117.9 (3)	C11—C10—C9	119.5 (3)
C13—N2—C9	118.6 (2)	C11—C10—H10	120.3
C13—N2—Cu1	114.89 (18)	C9—C10—H10	120.3
C9—N2—Cu1	126.25 (18)	C10—C11—C12	119.0 (3)
C18—N3—C14	118.9 (2)	C10—C11—H11A	120.5
C18—N3—Cu1	125.6 (2)	C12—C11—H11A	120.5
C14—N3—Cu1	115.52 (18)	C11—C12—C13	118.9 (3)
C1—O1—Cu1	108.99 (16)	C11—C12—H12A	120.5
C8—O3—Cu1^{i}	134.66 (17)	C13—C12—H12A	120.5
Cu1—O1W—H11	109 (2)	N2—C13—C12	121.9 (3)
Cu1—O1W—H12	116 (2)	N2—C13—C14	114.5 (2)
H11—O1W—H12	112 (2)	C12—C13—C14	123.6 (2)
H21—O2W—H22	109 (2)	N3—C14—C15	121.4 (3)
O2—C1—O1	124.0 (2)	N3—C14—C13	114.6 (2)
O2—C1—C2	118.2 (2)	C15—C14—C13	124.0 (3)
O1—C1—C2	117.7 (2)	C16—C15—C14	119.2 (3)
C3—C2—C7	120.2 (2)	C16—C15—H15	120.4
C3—C2—C1	116.7 (2)	C14—C15—H15	120.4
C7—C2—C1	123.1 (2)	C15—C16—C17	119.2 (3)
C4—C3—C2	121.8 (3)	C15—C16—H16	120.4
C4—C3—H3	119.1	C17—C16—H16	120.4
C2—C3—H3	119.1	C18—C17—C16	118.9 (3)
C3—C4—C5	119.3 (3)	C18—C17—H17	120.5
C3—C4—H4	120.3	C16—C17—H17	120.5
C5—C4—H4	120.3	N3—C18—C17	122.4 (3)
C6—C5—C4	118.8 (3)	N3—C18—H18	118.8
C6—C5—H5	120.6	C17—C18—H18	118.8
C4—C5—H5	120.6		

O1—Cu1—N2—C13	−164.61 (18)	C3—C2—C7—C8	176.7 (2)
O1W—Cu1—N2—C13	−51.0 (3)	C1—C2—C7—C8	−2.3 (4)
N3—Cu1—N2—C13	4.59 (18)	C5—C6—C7—C2	−1.3 (4)
O3^{i}—Cu1—N2—C13	97.54 (19)	N1—C6—C7—C2	178.2 (2)
O1—Cu1—N2—C9	9.4 (2)	C5—C6—C7—C8	−177.7 (2)
O1W—Cu1—N2—C9	123.1 (3)	N1—C6—C7—C8	1.8 (4)
N3—Cu1—N2—C9	178.6 (2)	Cu1^{i}—O3—C8—O4	−14.3 (4)
O3^{i}—Cu1—N2—C9	−88.4 (2)	Cu1^{i}—O3—C8—C7	166.26 (16)
O1—Cu1—N3—C18	−110.3 (4)	C2—C7—C8—O3	96.7 (3)
O1W—Cu1—N3—C18	−17.1 (2)	C6—C7—C8—O3	−87.1 (3)
N2—Cu1—N3—C18	179.0 (3)	C2—C7—C8—O4	−82.8 (3)
O3^{i}—Cu1—N3—C18	69.4 (2)	C6—C7—C8—O4	93.3 (3)
O1—Cu1—N3—C14	68.2 (5)	C13—N2—C9—C10	−0.5 (4)

O1W—Cu1—N3—C14	161.3 (2)	Cu1—N2—C9—C10	−174.3 (2)
N2—Cu1—N3—C14	−2.61 (19)	N2—C9—C10—C11	1.1 (5)
O3^{i}—Cu1—N3—C14	−112.15 (19)	C9—C10—C11—C12	−0.5 (5)
O1W—Cu1—O1—C1	−79.31 (17)	C10—C11—C12—C13	−0.7 (4)
N3—Cu1—O1—C1	13.5 (5)	C9—N2—C13—C12	−0.7 (4)
N2—Cu1—O1—C1	82.74 (17)	Cu1—N2—C13—C12	173.8 (2)
O3^{i}—Cu1—O1—C1	−166.23 (16)	C9—N2—C13—C14	179.8 (2)
Cu1—O1—C1—O2	−4.2 (3)	Cu1—N2—C13—C14	−5.7 (3)
Cu1—O1—C1—C2	177.93 (17)	C11—C12—C13—N2	1.3 (4)
O2—C1—C2—C3	−26.2 (4)	C11—C12—C13—C14	−179.3 (3)
O1—C1—C2—C3	151.8 (2)	C18—N3—C14—C15	−0.3 (4)
O2—C1—C2—C7	152.9 (2)	Cu1—N3—C14—C15	−178.9 (2)
O1—C1—C2—C7	−29.2 (4)	C18—N3—C14—C13	178.9 (2)
C7—C2—C3—C4	1.7 (4)	Cu1—N3—C14—C13	0.4 (3)
C1—C2—C3—C4	−179.2 (3)	N2—C13—C14—N3	3.5 (3)
C2—C3—C4—C5	−2.8 (5)	C12—C13—C14—N3	−176.0 (3)
C3—C4—C5—C6	1.7 (5)	N2—C13—C14—C15	−177.3 (3)
C4—C5—C6—C7	0.3 (4)	C12—C13—C14—C15	3.3 (4)
C4—C5—C6—N1	−179.2 (3)	N3—C14—C15—C16	0.6 (4)
O5—N1—C6—C5	−175.4 (3)	C13—C14—C15—C16	−178.6 (3)
O6—N1—C6—C5	3.8 (4)	C14—C15—C16—C17	−0.8 (5)
O5—N1—C6—C7	5.1 (4)	C15—C16—C17—C18	0.7 (5)
O6—N1—C6—C7	−175.7 (3)	C14—N3—C18—C17	0.3 (5)
C3—C2—C7—C6	0.3 (4)	Cu1—N3—C18—C17	178.7 (2)
C1—C2—C7—C6	−178.7 (2)	C16—C17—C18—N3	−0.5 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2w	0.83 (3)	1.85 (1)	2.660 (3)	166 (3)
O1w—H12···O4^{ii}	0.83 (3)	1.90 (1)	2.718 (3)	168 (3)
O2w—H21···O4	0.84 (3)	2.04 (2)	2.830 (3)	158 (3)
O2w—H22···O1^{i}	0.84 (3)	2.25 (2)	2.985 (3)	146 (3)
O2w—H22···O3^{i}	0.84 (3)	2.35 (3)	2.977 (3)	132 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1.