Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(2,2′-bipyridine-κ^2N,N')bis(4-iodobenzoato-κO)copper(II)

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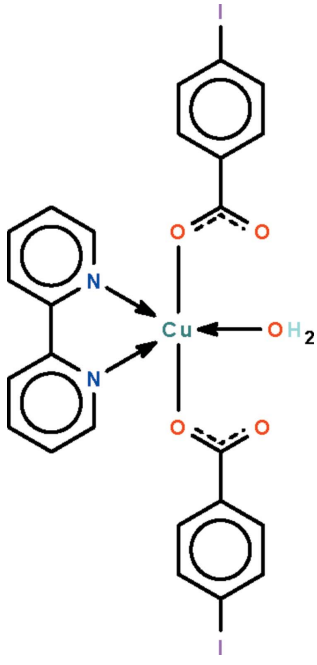
Received 27 October 2010; accepted 3 November 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.012 Å; R factor = 0.058; wR factor = 0.175; data-to-parameter ratio = 18.4.

The Cu^{II} atom in the title compound, $[Cu(C_7H_4IO_2)_2(C_{10}H_8N_2)(H_2O)]$, is N,N'-chelated by a 2,2′-bipyridine ligand and is coordinated by two monodentate carboxylate ions and a water molecule in a distorted square-pyramidal geometry. The apical site is occupied by one of the carboxylate O atoms. The water molecule forms intramolecular hydrogen bonds to the uncoordinated carboxyl O atoms. The crystal studied was a nonmerohedral twin with minor components in 0.381 (3) and 0.108 (2) proportions.

Related literature

For related copper carboxylate–2,2′-bipyridine adducts, see: He *et al.* (2007); Li *et al.* (2006); Liu *et al.* (2006); Yang *et al.* (1994).



Experimental

Crystal data

$[Cu(C_7H_4IO_2)_2(C_{10}H_8N_2)(H_2O)]$
M_r = 731.74
Monoclinic, $P2_1/c$
a = 13.0571 (2) Å
b = 16.0724 (2) Å
c = 11.9605 (2) Å
β = 103.298 (1)°
V = 2442.72 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.46 mm^{-1}
T = 100 K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*TWINABS*; Bruker, 2009)
T_{min} = 0.355, T_{max} = 0.745
33957 measured reflections
5698 independent reflections
4505 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.175
S = 1.08
5698 reflections
310 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.71 e Å^{-3}
$\Delta\rho_{min}$ = −1.69 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.982 (7)	Cu1—O3	2.216 (6)
Cu1—N2	2.009 (6)	Cu1—O1*W*	1.959 (5)
Cu1—O1	1.977 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2	0.84	1.79	2.560 (9)	152
O1w—H12···O4	0.84	1.79	2.575 (8)	154

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5068).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2*, *SAINT* and *TWINABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
He, X.-M., Li, C.-H., Yang, Y.-Q. & Li, W. (2007). *Chin. J. Struct. Chem.* **26**, 206–210.
Li, W., Li, C.-H., Yang, Y.-Q., Kuang, D.-Z. & Xu, W.-J. (2006). *Chin. J. Struct. Chem.* **25**, 616–620.
Liu, F.-Q., Wang, Q.-X., Jiao, K., Jian, F.-F., Liu, G.-Y. & Li, R.-X. (2006). *Inorg. Chim. Acta*, **359**, 1524–1530.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yang, R.-N., Wang, D.-M., Jin, D.-M., Wang, H.-Q. & Yang, Y. (1994). *Chin. J. Struct. Chem.* **13**, 45–47.

supporting information

Acta Cryst. (2010). E**66**, m1530 [https://doi.org/10.1107/S1600536810044995]

Aqua(2,2′-bipyridine-κ^2N,N')bis(4-iodobenzoato-κO)copper(II)

Mohamad Isa Mohamadin, Norbani Abdullah, Kong Mun Lo and Seik Weng Ng

S1. Comment

Copper(II) benzoate and its analogs form adducts with 2,2′-bipyridine. The copper benzoate homolog furnishes a water-coordinated adduct (Yang *et al.*, 1994), as does copper *p*-toluate (Li *et al.*, 2006; Liu *et al.*, 2006) and copper *o*-toluate (He *et al.*, 2007). The copper atom in $Cu(H_2O)(C_{10}H_8N_2)(C_7H_4IO_2)_2$ (Scheme I) is chelated by the *N*-heterocycle and is coordinated by two monodentate carboxylate ions and a water molecule in a square-pyramidal geometry (Fig. 1). The apical site is occupied by the O atom of the carboxylate unit. The crystal studied is a non-merohedral twin with minor components in a 0.381 (3) and 0.108 (2) proportion.

S2. Experimental

Copper acetate monohydrate (2.00 g, 10 mmol) and 4-iodobenzoic acid (4.96 g, 20 mmol) were heated in aqueous ethanol (1:1, 60 ml) for 1 h. The solvent was removed to give blue copper bis(4-iodobenzoate), which was isolated in 50% yield. The powder and 2,2′-bipyridine (0.77 g, 5 mmol) were dissolved in tetrahydrofuran. Crystals were isolated after several days.

S3. Refinement

H atoms were placed in calculated positions (C–H 0.95, O–H 0.84 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2 to 1.5U(C,O).

The final difference Fourier map had a peak and a hole in the vicinity of I2.

The crystal studied is a non-merohedral twin with minor components in a 38.1 (3) and 10.8 (2)% proportion. The twinned nature of the crystal structure adversely affected the quality of the diffraction measured, and this is reflected in the somewhat larger numbers in the weighting scheme.

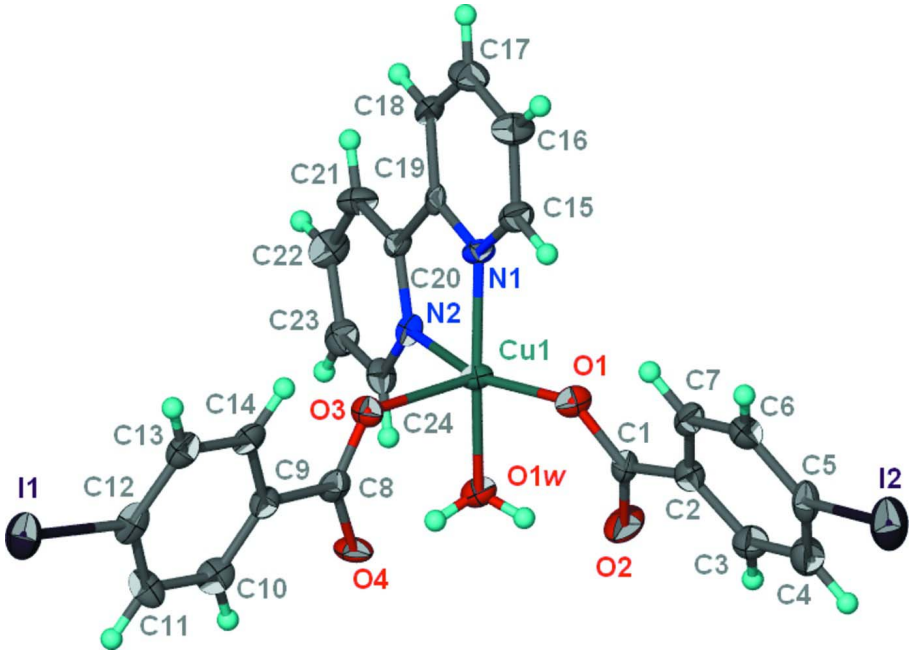


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Cu(H_2O)(C_{10}H_8N_2)(C_7H_4IO_2)_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$[Cu(C_7H_4IO_2)_2(C_{10}H_8N_2)(H_2O)]$
$M_r = 731.74$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.0571\ (2)$ Å
$b = 16.0724\ (2)$ Å
$c = 11.9605\ (2)$ Å
$\beta = 103.298\ (1)°$
$V = 2442.72\ (6)$ Å^3
$Z = 4$
$F(000) = 1404$
$D_x = 1.990$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1215 reflections
$\theta = 2.5–24.2°$
$\mu = 3.46$ mm^{-1}
$T = 100$ K
Cube, blue
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*TWINABS*; Bruker, 2009)
$T_{min} = 0.423$, $T_{max} = 0.423$
33957 measured reflections
5698 independent reflections
4505 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.0°$
$h = -15\rightarrow15$
$k = 0\rightarrow19$
$l = 0\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.175$
$S = 1.08$
5698 reflections
310 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
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 12.0788P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.71$ e Å^{-3}
$\Delta\rho_{min} = -1.69$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	1.52100 (5)	0.77933 (4)	0.96178 (5)	0.0307 (2)
I2	0.54254 (5)	1.06313 (4)	0.81444 (6)	0.0370 (2)
Cu1	0.88404 (8)	0.70624 (6)	0.44393 (8)	0.0165 (3)
O1	0.7975 (5)	0.7791 (3)	0.5186 (5)	0.0189 (13)
O2	0.7765 (5)	0.8878 (4)	0.3970 (6)	0.0319 (16)
O3	1.0368 (4)	0.7208 (3)	0.5695 (5)	0.0182 (12)
O4	1.0982 (5)	0.8248 (4)	0.4776 (5)	0.0220 (13)
O1W	0.9172 (5)	0.7943 (3)	0.3446 (5)	0.0203 (13)
H11	0.8773	0.8352	0.3455	0.030*
H12	0.9801	0.8092	0.3687	0.030*
N1	0.8380 (5)	0.6058 (4)	0.5151 (6)	0.0162 (15)
N2	0.9245 (5)	0.6191 (4)	0.3416 (5)	0.0144 (14)
C1	0.7637 (7)	0.8513 (5)	0.4846 (8)	0.0215 (19)
C2	0.7064 (7)	0.8978 (5)	0.5618 (7)	0.0209 (18)
C3	0.6627 (7)	0.9757 (5)	0.5274 (8)	0.024 (2)
H3	0.6656	0.9967	0.4540	0.029*
C4	0.6158 (7)	1.0224 (6)	0.5975 (8)	0.028 (2)
H4	0.5884	1.0759	0.5737	0.034*
C5	0.6090 (7)	0.9913 (5)	0.7019 (8)	0.0236 (19)
C6	0.6510 (7)	0.9127 (5)	0.7390 (8)	0.026 (2)
H6	0.6470	0.8919	0.8122	0.031*
C7	0.6977 (7)	0.8665 (5)	0.6682 (7)	0.0219 (19)
H7	0.7245	0.8128	0.6916	0.026*
C8	1.1036 (7)	0.7747 (5)	0.5605 (7)	0.0195 (18)
C9	1.2009 (7)	0.7822 (5)	0.6583 (7)	0.0171 (17)
C10	1.2850 (7)	0.8289 (5)	0.6483 (7)	0.0217 (19)
H10	1.2808	0.8612	0.5809	0.026*
C11	1.3773 (7)	0.8306 (5)	0.7346 (7)	0.0222 (19)
H11A	1.4365	0.8623	0.7263	0.027*
C12	1.3794 (7)	0.7842 (5)	0.8332 (7)	0.0216 (19)
C13	1.2941 (7)	0.7393 (5)	0.8471 (8)	0.0235 (19)
H13	1.2969	0.7096	0.9164	0.028*
C14	1.2052 (7)	0.7373 (5)	0.7612 (7)	0.0204 (18)
H14	1.1460	0.7059	0.7703	0.024*

C15	0.7940 (7)	0.6048 (5)	0.6056 (7)	0.0218 (19)
H15	0.7804	0.6566	0.6378	0.026*
C16	0.7670 (8)	0.5324 (5)	0.6550 (8)	0.025 (2)
H16	0.7364	0.5339	0.7198	0.030*
C17	0.7866 (7)	0.4578 (6)	0.6057 (8)	0.026 (2)
H17	0.7687	0.4068	0.6365	0.031*
C18	0.8320 (7)	0.4570 (5)	0.5122 (8)	0.0230 (19)
H18	0.8456	0.4059	0.4782	0.028*
C19	0.8573 (6)	0.5329 (5)	0.4690 (7)	0.0152 (17)
C20	0.9038 (6)	0.5399 (5)	0.3673 (7)	0.0166 (17)
C21	0.9213 (7)	0.4734 (5)	0.3003 (8)	0.026 (2)
H21	0.9065	0.4181	0.3200	0.031*
C22	0.9603 (8)	0.4886 (6)	0.2050 (7)	0.026 (2)
H22	0.9734	0.4439	0.1582	0.031*
C23	0.9802 (7)	0.5701 (5)	0.1779 (8)	0.024 (2)
H23	1.0054	0.5821	0.1112	0.029*
C24	0.9627 (6)	0.6336 (5)	0.2493 (7)	0.0195 (18)
H24	0.9784	0.6892	0.2320	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0258 (3)	0.0370 (4)	0.0256 (4)	0.0053 (3)	−0.0018 (2)	−0.0007 (2)
I2	0.0303 (4)	0.0424 (4)	0.0393 (4)	0.0066 (3)	0.0099 (3)	−0.0150 (3)
Cu1	0.0216 (6)	0.0126 (5)	0.0153 (5)	−0.0010 (4)	0.0045 (4)	0.0007 (4)
O1	0.026 (3)	0.016 (3)	0.015 (3)	0.000 (2)	0.007 (3)	−0.004 (2)
O2	0.039 (4)	0.029 (4)	0.032 (4)	0.010 (3)	0.017 (3)	0.017 (3)
O3	0.017 (3)	0.020 (3)	0.015 (3)	−0.002 (2)	0.000 (2)	0.000 (2)
O4	0.025 (3)	0.021 (3)	0.019 (3)	−0.007 (3)	0.003 (3)	0.008 (2)
O1W	0.025 (3)	0.017 (3)	0.018 (3)	0.000 (2)	0.002 (3)	0.001 (2)
N1	0.020 (4)	0.010 (3)	0.017 (4)	−0.003 (3)	0.000 (3)	−0.001 (3)
N2	0.016 (3)	0.017 (4)	0.008 (3)	0.003 (3)	0.000 (3)	0.001 (3)
C1	0.016 (4)	0.020 (5)	0.028 (5)	0.004 (3)	0.005 (4)	0.007 (4)
C2	0.017 (4)	0.020 (4)	0.025 (5)	−0.001 (3)	0.002 (4)	0.000 (3)
C3	0.025 (5)	0.023 (5)	0.026 (5)	0.000 (4)	0.008 (4)	0.004 (3)
C4	0.022 (5)	0.026 (5)	0.036 (6)	0.001 (4)	0.006 (4)	−0.003 (4)
C5	0.015 (4)	0.026 (5)	0.027 (5)	0.003 (4)	−0.001 (4)	−0.011 (4)
C6	0.021 (5)	0.022 (5)	0.036 (6)	−0.001 (4)	0.009 (4)	0.001 (4)
C7	0.017 (4)	0.017 (4)	0.027 (5)	0.001 (3)	−0.007 (4)	−0.002 (3)
C8	0.023 (5)	0.015 (4)	0.022 (5)	0.003 (4)	0.008 (4)	−0.004 (3)
C9	0.020 (4)	0.019 (4)	0.014 (4)	0.004 (3)	0.005 (3)	0.002 (3)
C10	0.030 (5)	0.024 (5)	0.013 (4)	0.002 (4)	0.009 (4)	0.000 (3)
C11	0.019 (4)	0.032 (5)	0.017 (4)	−0.005 (4)	0.007 (4)	−0.006 (3)
C12	0.029 (5)	0.022 (4)	0.015 (4)	0.009 (4)	0.007 (4)	−0.008 (3)
C13	0.026 (5)	0.019 (4)	0.025 (5)	0.005 (4)	0.004 (4)	−0.001 (3)
C14	0.025 (5)	0.012 (4)	0.024 (5)	0.004 (3)	0.006 (4)	−0.002 (3)
C15	0.024 (5)	0.017 (4)	0.024 (5)	0.000 (4)	0.004 (4)	−0.001 (3)
C16	0.034 (5)	0.023 (5)	0.019 (5)	−0.004 (4)	0.008 (4)	0.002 (3)

C17	0.028 (5)	0.027 (5)	0.023 (5)	−0.006 (4)	0.008 (4)	0.006 (4)
C18	0.019 (5)	0.013 (4)	0.037 (5)	0.003 (3)	0.006 (4)	0.003 (4)
C19	0.010 (4)	0.019 (4)	0.015 (4)	0.004 (3)	−0.002 (3)	0.004 (3)
C20	0.016 (4)	0.014 (4)	0.019 (5)	0.001 (3)	0.000 (3)	0.000 (3)
C21	0.031 (5)	0.017 (5)	0.029 (5)	−0.005 (4)	0.006 (4)	0.002 (3)
C22	0.035 (5)	0.023 (5)	0.020 (5)	0.002 (4)	0.007 (4)	−0.006 (4)
C23	0.023 (5)	0.028 (5)	0.020 (5)	0.002 (4)	0.002 (4)	0.004 (4)
C24	0.019 (4)	0.025 (5)	0.017 (5)	0.002 (4)	0.009 (4)	−0.001 (3)

Geometric parameters (Å, º)

I1—C12	2.117 (9)	C8—C9	1.521 (12)
I2—C5	2.106 (8)	C9—C10	1.358 (12)
Cu1—N1	1.982 (7)	C9—C14	1.416 (11)
Cu1—N2	2.009 (6)	C10—C11	1.395 (12)
Cu1—O1	1.977 (5)	C10—H10	0.9500
Cu1—O3	2.216 (6)	C11—C12	1.390 (12)
Cu1—O1W	1.959 (5)	C11—H11A	0.9500
O1—C1	1.275 (10)	C12—C13	1.369 (13)
O2—C1	1.246 (10)	C13—C14	1.363 (12)
O3—C8	1.251 (10)	C13—H13	0.9500
O4—C8	1.268 (10)	C14—H14	0.9500
O1W—H11	0.8400	C15—C16	1.387 (12)
O1W—H12	0.8400	C15—H15	0.9500
N1—C15	1.338 (11)	C16—C17	1.386 (12)
N1—C19	1.344 (10)	C16—H16	0.9500
N2—C24	1.332 (10)	C17—C18	1.380 (12)
N2—C20	1.351 (10)	C17—H17	0.9500
C1—C2	1.513 (12)	C18—C19	1.394 (11)
C2—C7	1.396 (12)	C18—H18	0.9500
C2—C3	1.397 (12)	C19—C20	1.484 (12)
C3—C4	1.369 (12)	C20—C21	1.386 (12)
C3—H3	0.9500	C21—C22	1.373 (12)
C4—C5	1.367 (13)	C21—H21	0.9500
C4—H4	0.9500	C22—C23	1.389 (13)
C5—C6	1.409 (12)	C22—H22	0.9500
C6—C7	1.370 (12)	C23—C24	1.383 (12)
C6—H6	0.9500	C23—H23	0.9500
C7—H7	0.9500	C24—H24	0.9500
O1W—Cu1—O1	94.3 (2)	C14—C9—C8	119.1 (7)
O1W—Cu1—N1	168.6 (3)	C9—C10—C11	121.6 (8)
O1—Cu1—N1	91.6 (3)	C9—C10—H10	119.2
O1W—Cu1—N2	90.5 (3)	C11—C10—H10	119.2
O1—Cu1—N2	161.0 (3)	C12—C11—C10	117.5 (8)
N1—Cu1—N2	80.9 (3)	C12—C11—H11A	121.3
O1W—Cu1—O3	92.6 (2)	C10—C11—H11A	121.3
O1—Cu1—O3	98.7 (2)	C13—C12—C11	121.9 (8)

N1—Cu1—O3	96.3 (2)	C13—C12—I1	119.4 (6)
N2—Cu1—O3	99.5 (2)	C11—C12—I1	118.6 (7)
C1—O1—Cu1	126.0 (5)	C14—C13—C12	119.8 (8)
C8—O3—Cu1	123.5 (5)	C14—C13—H13	120.1
Cu1—O1W—H11	109.5	C12—C13—H13	120.1
Cu1—O1W—H12	109.5	C13—C14—C9	120.0 (8)
H11—O1W—H12	109.5	C13—C14—H14	120.0
C15—N1—C19	118.6 (7)	C9—C14—H14	120.0
C15—N1—Cu1	125.9 (5)	N1—C15—C16	123.6 (8)
C19—N1—Cu1	115.5 (5)	N1—C15—H15	118.2
C24—N2—C20	119.1 (7)	C16—C15—H15	118.2
C24—N2—Cu1	125.7 (6)	C17—C16—C15	117.1 (8)
C20—N2—Cu1	115.1 (5)	C17—C16—H16	121.5
O2—C1—O1	126.4 (8)	C15—C16—H16	121.5
O2—C1—C2	117.5 (7)	C18—C17—C16	120.6 (8)
O1—C1—C2	116.1 (7)	C18—C17—H17	119.7
C7—C2—C3	118.5 (8)	C16—C17—H17	119.7
C7—C2—C1	122.2 (8)	C17—C18—C19	118.3 (8)
C3—C2—C1	119.3 (7)	C17—C18—H18	120.9
C4—C3—C2	121.4 (8)	C19—C18—H18	120.9
C4—C3—H3	119.3	N1—C19—C18	121.9 (7)
C2—C3—H3	119.3	N1—C19—C20	114.9 (7)
C5—C4—C3	119.4 (9)	C18—C19—C20	123.2 (7)
C5—C4—H4	120.3	N2—C20—C21	121.8 (7)
C3—C4—H4	120.3	N2—C20—C19	113.5 (7)
C4—C5—C6	120.9 (8)	C21—C20—C19	124.6 (7)
C4—C5—I2	120.5 (7)	C22—C21—C20	119.0 (8)
C6—C5—I2	118.6 (6)	C22—C21—H21	120.5
C7—C6—C5	119.2 (8)	C20—C21—H21	120.5
C7—C6—H6	120.4	C21—C22—C23	119.1 (8)
C5—C6—H6	120.4	C21—C22—H22	120.4
C6—C7—C2	120.6 (8)	C23—C22—H22	120.4
C6—C7—H7	119.7	C24—C23—C22	119.1 (8)
C2—C7—H7	119.7	C24—C23—H23	120.5
O3—C8—O4	126.4 (8)	C22—C23—H23	120.5
O3—C8—C9	117.7 (7)	N2—C24—C23	121.9 (8)
O4—C8—C9	115.9 (7)	N2—C24—H24	119.0
C10—C9—C14	119.1 (8)	C23—C24—H24	119.0
C10—C9—C8	121.7 (7)		

O1W—Cu1—O1—C1	13.0 (7)	Cu1—O3—C8—C9	174.9 (5)
N1—Cu1—O1—C1	−157.2 (7)	O3—C8—C9—C10	169.1 (8)
N2—Cu1—O1—C1	−91.2 (10)	O4—C8—C9—C10	−11.3 (11)
O3—Cu1—O1—C1	106.2 (7)	O3—C8—C9—C14	−9.0 (11)
O1W—Cu1—O3—C8	2.8 (6)	O4—C8—C9—C14	170.5 (7)
O1—Cu1—O3—C8	−91.9 (6)	C14—C9—C10—C11	3.1 (12)
N1—Cu1—O3—C8	175.6 (6)	C8—C9—C10—C11	−175.0 (7)
N2—Cu1—O3—C8	93.8 (6)	C9—C10—C11—C12	−1.6 (12)

O1W—Cu1—N1—C15	−138.5 (12)	C10—C11—C12—C13	−1.0 (12)
O1—Cu1—N1—C15	−17.7 (7)	C10—C11—C12—I1	176.3 (6)
N2—Cu1—N1—C15	179.8 (7)	C11—C12—C13—C14	2.0 (12)
O3—Cu1—N1—C15	81.2 (7)	I1—C12—C13—C14	−175.3 (6)
O1W—Cu1—N1—C19	44.0 (17)	C12—C13—C14—C9	−0.5 (12)
O1—Cu1—N1—C19	164.8 (6)	C10—C9—C14—C13	−2.1 (12)
N2—Cu1—N1—C19	2.3 (6)	C8—C9—C14—C13	176.1 (7)
O3—Cu1—N1—C19	−96.3 (6)	C19—N1—C15—C16	0.1 (13)
O1W—Cu1—N2—C24	2.9 (7)	Cu1—N1—C15—C16	−177.3 (7)
O1—Cu1—N2—C24	107.7 (9)	N1—C15—C16—C17	−0.6 (14)
N1—Cu1—N2—C24	175.3 (7)	C15—C16—C17—C18	0.6 (14)
O3—Cu1—N2—C24	−89.8 (7)	C16—C17—C18—C19	0.0 (14)
O1W—Cu1—N2—C20	−172.7 (6)	C15—N1—C19—C18	0.5 (12)
O1—Cu1—N2—C20	−68.0 (10)	Cu1—N1—C19—C18	178.2 (6)
N1—Cu1—N2—C20	−0.3 (6)	C15—N1—C19—C20	178.5 (7)
O3—Cu1—N2—C20	94.6 (6)	Cu1—N1—C19—C20	−3.8 (9)
Cu1—O1—C1—O2	2.1 (13)	C17—C18—C19—N1	−0.6 (13)
Cu1—O1—C1—C2	−175.2 (5)	C17—C18—C19—C20	−178.4 (8)
O2—C1—C2—C7	−172.9 (8)	C24—N2—C20—C21	0.1 (12)
O1—C1—C2—C7	4.7 (12)	Cu1—N2—C20—C21	176.0 (7)
O2—C1—C2—C3	5.4 (13)	C24—N2—C20—C19	−177.5 (7)
O1—C1—C2—C3	−177.0 (8)	Cu1—N2—C20—C19	−1.5 (9)
C7—C2—C3—C4	2.5 (13)	N1—C19—C20—N2	3.5 (11)
C1—C2—C3—C4	−175.9 (9)	C18—C19—C20—N2	−178.6 (8)
C2—C3—C4—C5	−1.8 (14)	N1—C19—C20—C21	−174.0 (8)
C3—C4—C5—C6	1.1 (14)	C18—C19—C20—C21	4.0 (14)
C3—C4—C5—I2	177.7 (7)	N2—C20—C21—C22	−0.3 (14)
C4—C5—C6—C7	−1.1 (13)	C19—C20—C21—C22	176.9 (8)
I2—C5—C6—C7	−177.8 (7)	C20—C21—C22—C23	−0.6 (14)
C5—C6—C7—C2	1.7 (13)	C21—C22—C23—C24	1.6 (14)
C3—C2—C7—C6	−2.4 (13)	C20—N2—C24—C23	1.1 (13)
C1—C2—C7—C6	175.9 (8)	Cu1—N2—C24—C23	−174.4 (6)
Cu1—O3—C8—O4	−4.6 (12)	C22—C23—C24—N2	−1.9 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2	0.84	1.79	2.560 (9)	152
O1w—H12···O4	0.84	1.79	2.575 (8)	154