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catena-Poly[[aqua{4-[*N*′-(2,4-dioxo-3-pentylidene)hydrazino]benzoato}-copper(II)]-μ-acetato]

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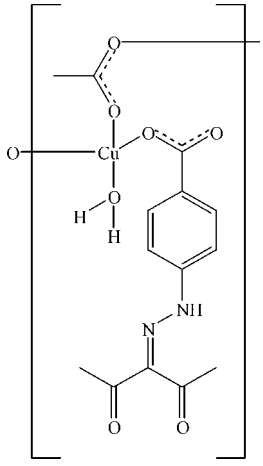
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.065; wR factor = 0.219; data-to-parameter ratio = 18.7.

In the title compound, $[Cu(CH_3CO_2)(C_{12}H_{11}N_2O_4)(H_2O)]_n$, the Cu^{II} cation is tetracoordinated by three carboxylate O atoms from one 4-[*N*′-(2,4-dioxo-3-pentylidene)hydrazino]-benzoate ligand and two acetate bridges, and by one water molecule. The acetate bridges link adjacent Cu^{II} cations, forming a chain. The crystal structure involves O—H···O hydrogen bonds.

Related literature

For uses of carboxylic acids in materials science, see: Church & Halvorson (1959). For uses in biological systems, see: Chung *et al.* (1971); Okabe & Oya (2000); Serre *et al.* (2005); Pocker & Fong (1980); Scapin *et al.* (1997); Kim *et al.* (2001).



Experimental

Crystal data

$[Cu(C_2H_3O_2)(C_{12}H_{11}N_2O_4)(H_2O)]$
M_r = 387.83
Monoclinic, $P2_1/c$
a = 8.106 (2) Å
b = 23.918 (4) Å
c = 8.946 (2) Å
β = 106.90 (3)°
V = 1659.5 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 293 (2) K
0.43 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.594, T_{max} = 0.755
8654 measured reflections
4235 independent reflections
2693 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.219
S = 1.00
4235 reflections
226 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −1.73 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.94 (5)	1.90 (5)	2.617 (5)	132 (4)
O7—H7A···O1^{ii}	0.84 (4)	1.91 (4)	2.739 (4)	168 (5)
O7—H7B···O4^{iii}	0.84 (5)	2.00 (3)	2.774 (5)	153 (6)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2197).

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Acta Cryst. (2008). E**64**, m929 [doi:10.1107/S1600536808016073]

catena-Poly[[aqua{4-[*N*′-(2,4-dioxo-3-pentylidene)hydrazino]benzoato}copper(II)]-μ-acetato]

Lujiang Hao, Chunhua Mu and Ridong Wang

S1. Comment

In recent years, carboxylates have been widely used as polydentate ligands, which can coordinate to transition or rare earth ions yielding complexes with interesting properties that are useful in materials science (Church & Halvorson, 1959; Chung *et al.*, 1971) and in biological systems (Okabe & Oya, 2000; Serre *et al.*, 2005; Pocker & Fong, 1980; Scapin *et al.*, 1997). For example, Kim *et al.* (2001) focused on the syntheses of transition metal complexes containing benzenecarboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal dicarboxylate complexes motivated us to pursue synthetic strategies for these compounds, using sodium 4-(2-(diacetylmethylene)hydrazino)benzoate as a polydentate ligand. Here we report the synthesis and X-ray crystal structure analysis of the title compound. The asymmetric unit of the title compound is shown in Fig. 1. The copper(II) cation is tetracoordinated by three carboxylate oxygen atoms from one 2,4-dioxo-3-pentylidene)hydrazino]benzoate ligand and two acetate bridges, and by one water molecule. The acetate bridges link adjacent copper(II) cations, forming a chain, shown in Fig. 2. The Cu—O bond distances are in the range 1.970 (4)–2.031 (4) Å. The packing involves O—H···O hydrogen bonds, with O···O in the range 2.744 (5)–3.058 (6) Å, as shown in Fig. 3.

S2. Experimental

A mixture of copper(II) acetate (0.5 mmol), 4-(2-(diacetylmethylene)hydrazino)benzoic acid (0.5 mmol), water (8 ml) and ethanol (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for three days. Colorless crystals were obtained after cooling to room temperature with a yield of 27%. Anal. Calc. for $C_{14}H_{15}CuN_2O_7$: C 43.43, H 3.88, N 7.24%; Found: C 43.36, H 3.79, N 7.16%.

S3. Refinement

The H atoms of the water molecule were located in a difference density map and were refined with distance restraints H···H = 1.38 (1) Å, O—H = 0.84 (1) Å, and with U_{iso}(H) = 1.2U_{eq}(O). The N-bound H atom was also located in a map, and was refined with no positional restraints and with U_{iso}(H) = 1.2U_{eq}(N). All other H atoms were placed in calculated positions with a C—H bond distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

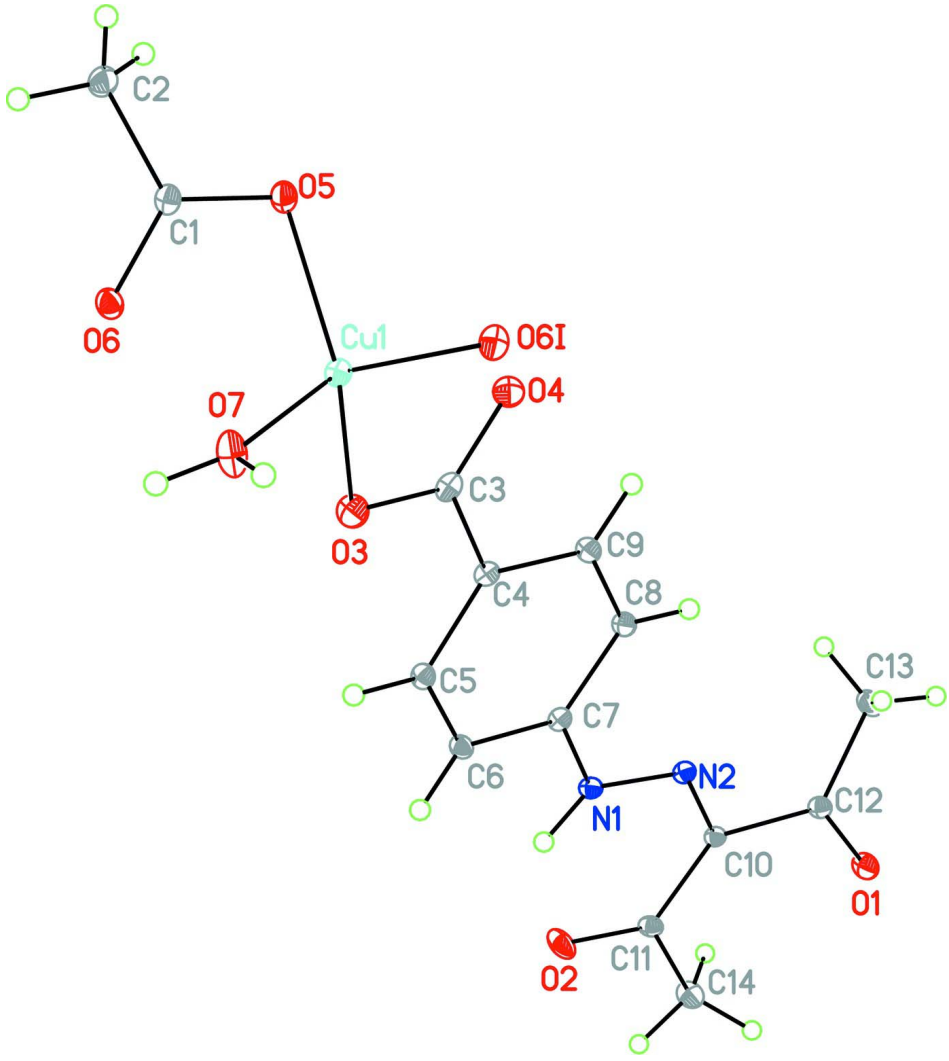

Figure 1

A segment of the polymeric structure of (I), showing the atomic numbering scheme and 30% probability displacement ellipsoids. [Symmetry code: (I), *x*, 3/2 - *y*, *z* - 1/2.]

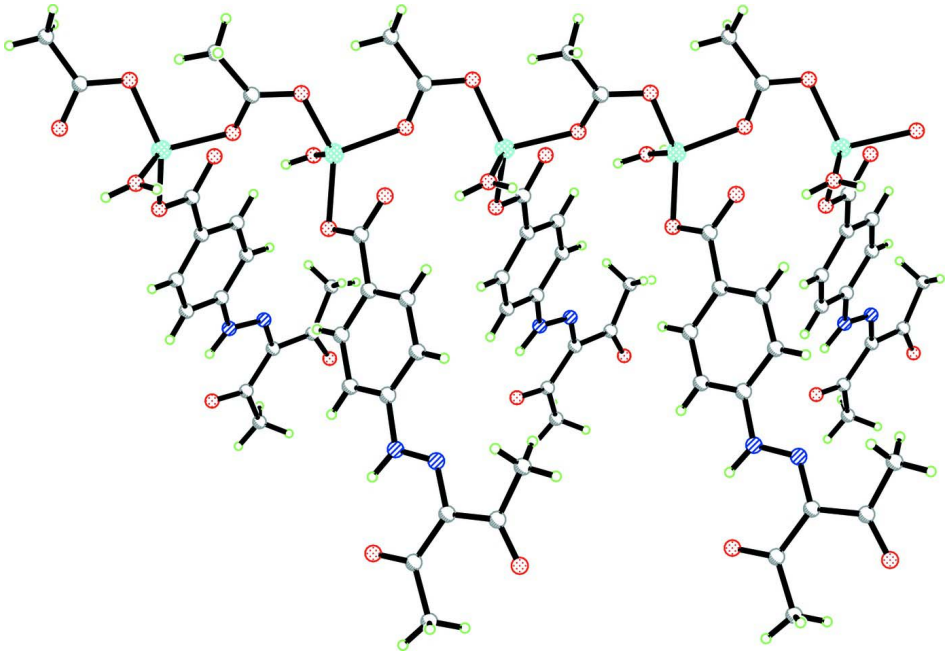

Figure 2

One-dimensional chain of (I).

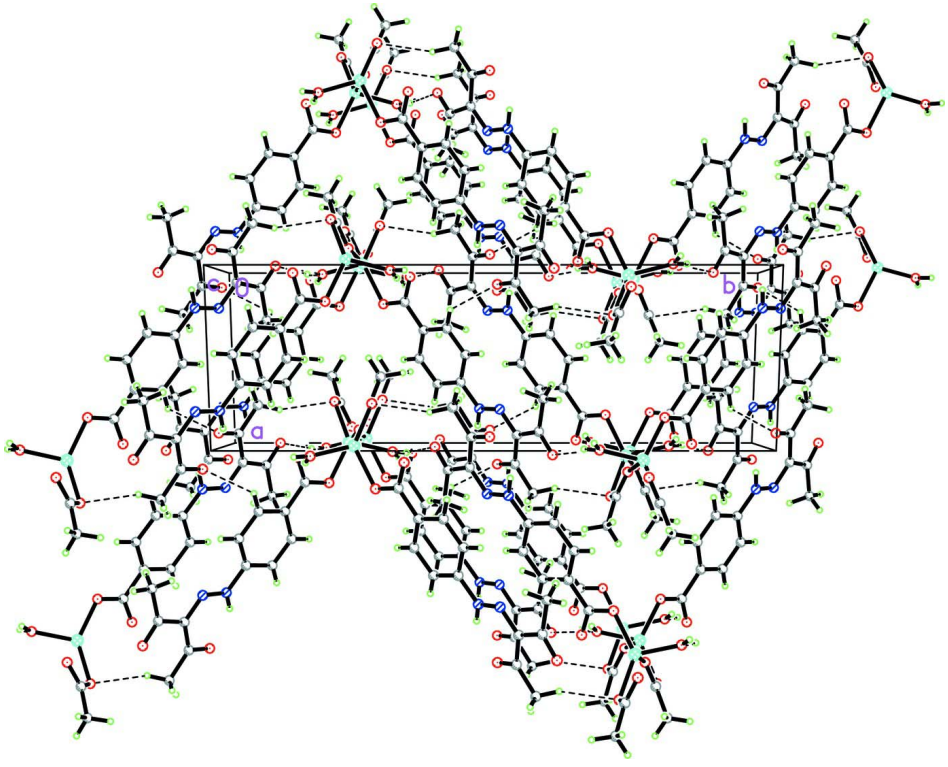

Figure 3

The packing of (I), with hydrogen bonds shown as dashed lines.

catena-Poly[[aqua{4-[_N_′-(2,4-dioxo-3- pentylidene)hydrazino]benzoato}copper(II)]-μ-acetato]

Crystal data

$[Cu(C_2H_3O_2)(C_{12}H_{11}N_2O_4)(H_2O)]$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.106$ (2) Å
$b = 23.918$ (4) Å
$c = 8.946$ (2) Å
$\beta = 106.90$ (3)°
$V = 1659.5$ (6) Å^3
$Z = 4$
$F(000) = 796$
$D_x = 1.552$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4235 reflections
$\theta = 1.7$–$28.8°$
$\mu = 1.35$ mm^{-1}
$T = 293$ K
Block, blue
0.43 × 0.28 × 0.22 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, 2004)
$T_{min} = 0.594$, $T_{max} = 0.755$
8654 measured reflections
4235 independent reflections
2693 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.8°$, $\theta_{min} = 1.7°$
$h = -10 \rightarrow 9$
$k = -31 \rightarrow 29$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.219$
$S = 1.00$
4235 reflections
226 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.167P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -1.73$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	−0.04150 (6)	0.25987 (2)	0.28607 (6)	0.0311 (2)
C1	−0.2534 (6)	0.28239 (16)	−0.0029 (5)	0.0339 (8)
C2	−0.4039 (6)	0.2997 (2)	−0.1400 (5)	0.0490 (11)

H2A	−0.3776	0.2918	−0.2358	0.073*
H2B	−0.4245	0.3390	−0.1337	0.073*
H2C	−0.5049	0.2793	−0.1375	0.073*
C3	0.1783 (5)	0.33727 (16)	0.4174 (5)	0.0340 (8)
C4	0.3381 (5)	0.37225 (15)	0.4810 (4)	0.0290 (8)
C5	0.4965 (5)	0.36320 (16)	0.4439 (5)	0.0326 (8)
H5A	0.5036	0.3340	0.3773	0.039*
C6	0.6407 (5)	0.39724 (16)	0.5056 (5)	0.0331 (8)
H6A	0.7423	0.3912	0.4796	0.040*
C7	0.6292 (5)	0.43991 (15)	0.6058 (4)	0.0299 (8)
C8	0.4760 (5)	0.44926 (16)	0.6466 (5)	0.0333 (8)
H8A	0.4712	0.4778	0.7158	0.040*
C9	0.3298 (5)	0.41525 (16)	0.5824 (5)	0.0332 (8)
H9A	0.2283	0.4217	0.6082	0.040*
C10	0.9194 (5)	0.54195 (16)	0.8363 (4)	0.0281 (7)
C11	1.0841 (5)	0.53851 (17)	0.7897 (5)	0.0346 (8)
C12	0.8959 (5)	0.58020 (16)	0.9595 (5)	0.0339 (8)
C13	0.7155 (6)	0.5879 (3)	0.9759 (7)	0.0562 (14)
H13A	0.7201	0.6133	1.0600	0.084*
H13B	0.6720	0.5524	0.9978	0.084*
H13C	0.6409	0.6027	0.8804	0.084*
C14	1.2423 (6)	0.5712 (2)	0.8705 (6)	0.0480 (11)
H14A	1.3319	0.5631	0.8233	0.072*
H14B	1.2801	0.5610	0.9790	0.072*
H14C	1.2164	0.6104	0.8612	0.072*
N1	0.7769 (4)	0.47437 (13)	0.6639 (4)	0.0306 (7)
H1	0.872 (6)	0.471 (2)	0.625 (5)	0.037*
N2	0.7779 (4)	0.51093 (13)	0.7725 (4)	0.0307 (7)
O1	1.0199 (4)	0.60409 (14)	1.0486 (4)	0.0493 (8)
O2	1.0905 (4)	0.50681 (17)	0.6823 (5)	0.0599 (11)
O3	0.1881 (4)	0.29684 (14)	0.3292 (4)	0.0511 (8)
O4	0.0403 (4)	0.34837 (14)	0.4497 (4)	0.0456 (8)
O5	−0.2621 (4)	0.28883 (13)	0.1365 (3)	0.0411 (7)
O6	−0.1154 (5)	0.26235 (12)	−0.0240 (4)	0.0424 (8)
O7	0.0168 (6)	0.18300 (14)	0.2414 (4)	0.0566 (10)
H7A	0.019 (8)	0.1569 (15)	0.305 (5)	0.068*
H7B	0.056 (7)	0.172 (2)	0.169 (4)	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0339 (4)	0.0265 (3)	0.0328 (4)	−0.00674 (17)	0.0093 (2)	−0.00117 (17)
C1	0.046 (2)	0.0210 (17)	0.033 (2)	0.0006 (15)	0.0104 (18)	−0.0006 (15)
C2	0.051 (3)	0.052 (3)	0.038 (2)	0.014 (2)	0.005 (2)	0.001 (2)
C3	0.040 (2)	0.0279 (19)	0.031 (2)	−0.0096 (15)	0.0056 (17)	0.0025 (15)
C4	0.0317 (18)	0.0214 (16)	0.0314 (19)	−0.0037 (13)	0.0054 (15)	0.0024 (14)
C5	0.038 (2)	0.0241 (17)	0.034 (2)	−0.0007 (15)	0.0091 (16)	−0.0046 (15)
C6	0.034 (2)	0.0295 (19)	0.037 (2)	0.0014 (15)	0.0118 (17)	−0.0041 (16)

C7	0.034 (2)	0.0225 (17)	0.031 (2)	−0.0020 (14)	0.0057 (16)	0.0002 (14)
C8	0.034 (2)	0.0267 (18)	0.038 (2)	−0.0027 (14)	0.0083 (17)	−0.0081 (15)
C9	0.033 (2)	0.0284 (19)	0.040 (2)	−0.0043 (15)	0.0126 (17)	−0.0059 (16)
C10	0.0255 (17)	0.0255 (17)	0.0309 (19)	−0.0021 (13)	0.0044 (15)	−0.0037 (14)
C11	0.0299 (19)	0.0279 (18)	0.044 (2)	0.0012 (15)	0.0082 (17)	−0.0040 (17)
C12	0.034 (2)	0.0268 (18)	0.040 (2)	0.0015 (15)	0.0088 (17)	−0.0029 (16)
C13	0.040 (3)	0.073 (4)	0.057 (3)	−0.001 (2)	0.016 (2)	−0.027 (3)
C14	0.037 (2)	0.046 (3)	0.062 (3)	−0.0148 (19)	0.017 (2)	−0.017 (2)
N1	0.0272 (15)	0.0255 (15)	0.0365 (18)	−0.0016 (12)	0.0054 (14)	−0.0046 (13)
N2	0.0315 (16)	0.0253 (15)	0.0326 (17)	−0.0011 (12)	0.0052 (14)	−0.0024 (13)
O1	0.0426 (17)	0.0464 (18)	0.057 (2)	−0.0065 (14)	0.0121 (15)	−0.0261 (16)
O2	0.0423 (18)	0.064 (2)	0.079 (3)	−0.0128 (17)	0.0269 (19)	−0.042 (2)
O3	0.0478 (19)	0.0438 (18)	0.061 (2)	−0.0139 (15)	0.0139 (16)	−0.0174 (16)
O4	0.0409 (18)	0.0461 (17)	0.0514 (19)	−0.0123 (13)	0.0162 (15)	−0.0021 (15)
O5	0.0487 (18)	0.0426 (17)	0.0334 (16)	0.0028 (14)	0.0141 (14)	−0.0007 (13)
O6	0.0505 (19)	0.0400 (17)	0.0382 (18)	0.0109 (13)	0.0152 (15)	0.0012 (13)
O7	0.105 (3)	0.0278 (17)	0.047 (2)	0.0048 (17)	0.037 (2)	0.0062 (14)

Geometric parameters (Å, º)

Cu1—O7	1.968 (4)	C8—C9	1.415 (5)
Cu1—O3	1.994 (3)	C8—H8A	0.9300
Cu1—O5	2.020 (3)	C9—H9A	0.9300
Cu1—O6^{i}	2.030 (3)	C10—N2	1.346 (5)
C1—O6	1.281 (5)	C10—C12	1.486 (5)
C1—O5	1.278 (5)	C10—C11	1.513 (5)
C1—C2	1.515 (6)	C11—O2	1.236 (5)
C2—H2A	0.9600	C11—C14	1.496 (6)
C2—H2B	0.9600	C12—O1	1.228 (5)
C2—H2C	0.9600	C12—C13	1.522 (6)
C3—O4	1.262 (5)	C13—H13A	0.9600
C3—O3	1.265 (5)	C13—H13B	0.9600
C3—C4	1.508 (5)	C13—H13C	0.9600
C4—C9	1.386 (5)	C14—H14A	0.9600
C4—C5	1.433 (5)	C14—H14B	0.9600
C5—C6	1.400 (5)	C14—H14C	0.9600
C5—H5A	0.9300	N1—N2	1.305 (4)
C6—C7	1.379 (5)	N1—H1	0.94 (5)
C6—H6A	0.9300	O6—Cu1^{ii}	2.030 (3)
C7—C8	1.410 (5)	O7—H7A	0.84 (4)
C7—N1	1.422 (5)	O7—H7B	0.84 (5)
O7—Cu1—O3	100.84 (16)	C4—C9—H9A	120.1
O7—Cu1—O5	113.86 (16)	C8—C9—H9A	120.1
O3—Cu1—O5	124.96 (15)	N2—C10—C12	112.1 (3)
O7—Cu1—O6^{i}	94.12 (13)	N2—C10—C11	124.4 (3)
O3—Cu1—O6^{i}	116.10 (15)	C12—C10—C11	123.5 (3)
O5—Cu1—O6^{i}	102.99 (13)	O2—C11—C14	118.2 (4)

O6—C1—O5	119.2 (4)	O2—C11—C10	119.1 (4)
O6—C1—C2	121.0 (4)	C14—C11—C10	122.7 (4)
O5—C1—C2	119.8 (4)	O1—C12—C10	120.7 (4)
C1—C2—H2A	109.5	O1—C12—C13	120.6 (4)
C1—C2—H2B	109.5	C10—C12—C13	118.7 (4)
H2A—C2—H2B	109.5	C12—C13—H13A	109.4
C1—C2—H2C	109.5	C12—C13—H13B	109.5
H2A—C2—H2C	109.5	H13A—C13—H13B	109.5
H2B—C2—H2C	109.5	C12—C13—H13C	109.5
O4—C3—O3	121.6 (4)	H13A—C13—H13C	109.5
O4—C3—C4	121.2 (4)	H13B—C13—H13C	109.5
O3—C3—C4	117.2 (4)	C11—C14—H14A	109.4
C9—C4—C5	118.7 (3)	C11—C14—H14B	109.5
C9—C4—C3	117.3 (3)	H14A—C14—H14B	109.5
C5—C4—C3	123.9 (3)	C11—C14—H14C	109.5
C6—C5—C4	121.5 (3)	H14A—C14—H14C	109.5
C6—C5—H5A	119.2	H14B—C14—H14C	109.5
C4—C5—H5A	119.2	N2—N1—C7	118.9 (3)
C7—C6—C5	118.7 (3)	N2—N1—H1	120 (3)
C7—C6—H6A	120.7	C7—N1—H1	121 (3)
C5—C6—H6A	120.6	N1—N2—C10	120.3 (3)
C6—C7—C8	121.1 (4)	C3—O3—Cu1	103.6 (3)
C6—C7—N1	117.2 (3)	C1—O5—Cu1	108.4 (3)
C8—C7—N1	121.6 (3)	C1—O6—Cu1^{ii}	134.8 (3)
C7—C8—C9	120.0 (4)	Cu1—O7—H7A	121 (3)
C7—C8—H8A	120.0	Cu1—O7—H7B	127 (3)
C9—C8—H8A	120.0	H7A—O7—H7B	110.9 (18)
C4—C9—C8	119.9 (3)		

O4—C3—C4—C9	3.1 (6)	N2—C10—C12—C13	−11.4 (6)
O3—C3—C4—C9	−177.6 (4)	C11—C10—C12—C13	168.9 (4)
O4—C3—C4—C5	−177.5 (4)	C6—C7—N1—N2	−172.2 (4)
O3—C3—C4—C5	1.8 (6)	C8—C7—N1—N2	8.7 (5)
C9—C4—C5—C6	−1.1 (6)	C7—N1—N2—C10	176.2 (3)
C3—C4—C5—C6	179.6 (4)	C12—C10—N2—N1	−178.9 (3)
C4—C5—C6—C7	0.8 (6)	C11—C10—N2—N1	0.8 (6)
C5—C6—C7—C8	0.3 (6)	O4—C3—O3—Cu1	−4.6 (5)
C5—C6—C7—N1	−178.8 (4)	C4—C3—O3—Cu1	176.2 (3)
C6—C7—C8—C9	−1.2 (6)	O7—Cu1—O3—C3	−154.1 (3)
N1—C7—C8—C9	177.9 (4)	O5—Cu1—O3—C3	76.3 (3)
C5—C4—C9—C8	0.2 (6)	O6^{i}—Cu1—O3—C3	−54.0 (3)
C3—C4—C9—C8	179.6 (4)	O6—C1—O5—Cu1	−2.5 (4)
C7—C8—C9—C4	0.9 (6)	C2—C1—O5—Cu1	178.9 (3)
N2—C10—C11—O2	2.7 (6)	O7—Cu1—O5—C1	−53.0 (3)
C12—C10—C11—O2	−177.6 (4)	O3—Cu1—O5—C1	71.1 (3)
N2—C10—C11—C14	−176.0 (4)	O6^{i}—Cu1—O5—C1	−153.5 (3)
C12—C10—C11—C14	3.7 (6)	O5—C1—O6—Cu1^{ii}	175.8 (3)

N2—C10—C12—O1	166.9 (4)	C2—C1—O6—Cu1^{ii}	−5.7 (6)
C11—C10—C12—O1	−12.8 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.94 (5)	1.90 (5)	2.617 (5)	132 (4)
O7—H7*A*···O1^{iii}	0.84 (4)	1.91 (4)	2.739 (4)	168 (5)
O7—H7*B*···O4^{ii}	0.84 (5)	2.00 (3)	2.774 (5)	153 (6)

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