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Aqua(3-formyl-2-oxidobenzoato-κ^2O^1,O^2)(1,10-phenanthroline-κ^2N,N')copper(II) methanol solvate

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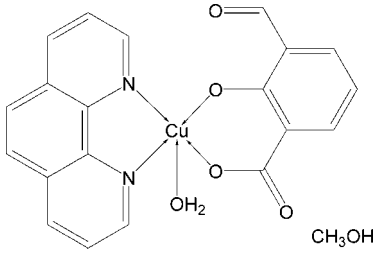
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.101; data-to-parameter ratio = 12.2.

In the structure of the title complex, $[Cu(C_8H_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot CH_4O$, the Cu^{II} ion is pentacoordinated in a tetragonal–pyramidal geometry, with two O atoms of the 3-formyl-2-oxidobenzoate (3-formylsalicylate) anion and two N atoms of 1,10-phenanthroline occupying the basal plane, and a water O atom located at the apical site. The structure displays O—H···O hydrogen bonding.

Related literature

For related literature, see: Erxleben & Schumacher (2001); Ma *et al.* (2007); Akitsu & Einaga (2006); Yu, Cui *et al.* (2007); Yu, Hao *et al.* (2006); Costes *et al.* (2004); Karmakar *et al.* (2005).



Experimental

Crystal data

$[Cu(C_8H_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot CH_4O$
M_r = 457.91
Triclinic, $P\overline{1}$
a = 8.6714 (11) Å
b = 10.3895 (13) Å
c = 11.7617 (14) Å
α = 115.125 (2)°
β = 95.859 (2)°
γ = 93.589 (2)°
V = 947.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 296 (2) K
0.21 × 0.16 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
4953 measured reflections
3336 independent reflections
2336 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.100
S = 0.94
3336 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1*W*	2.348 (3)	Cu1—N1	2.016 (3)
Cu1—O2	1.898 (2)	Cu1—N2	2.011 (3)
Cu1—O3	1.898 (2)		
O1*W*—Cu1—O2	93.40 (11)	O2—Cu1—N1	88.77 (11)
O1*W*—Cu1—O3	90.04 (10)	O2—Cu1—N2	166.01 (11)
O1*W*—Cu1—N1	96.50 (11)	O3—Cu1—N1	172.59 (11)
O1*W*—Cu1—N2	97.69 (10)	O3—Cu1—N2	94.17 (11)
O2—Cu1—O3	94.32 (10)	N1—Cu1—N2	81.55 (11)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O1^{i}	0.82	1.89	2.703 (4)	171
O1*W*—H1*WB*···O5^{ii}	0.85	1.93	2.747 (4)	162
O1*W*—H1*WA*···O4^{iii}	0.85	2.00	2.844 (4)	170

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); 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: KJ2080).

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supplementary materials

Acta Cryst. (2008). E**64**, m294 [**doi:10.1107/S1600536807067967**]

Aqua(3-formyl-2-oxidobenzoato-κ^2O^1,O^2)(1,10-phenanthroline-κ^2N,N')copper(II) methanol solvate

W. Zhang, Q. Cui, L. Chang and Z. Yu

Comment

The Schiff bases of 3-formylsalicylic acid with diamines have been studied for many years and their binuclear complexes have been intensively investigated in view of the interesting magnetic interaction between the bridged metals (Akitsu & Einaga, 2006; Karmakar *et al.*, 2005; Costes *et al.*, 2004). Recently some complexes with the schiff base of 3-formysalicylic acid and monoamines (Yu, Hao *et al.*, 2006; Yu, Cui *et al.*, 2007; Erxleben & Schumacher, 2001; Ma *et al.*, 2007) have also been reported. But to our knowledge, complexes using 3-formylsalicylic acid directly as ligand have received much less attention. Here we synthesized a multicomponent complex, containing 3-formylsalicylic acid and 1,10-phenanthroline.

The Cu^{II} ion is coordinated in distorted square pyramid, where the basal plane is formed by NNOO atoms coming from 1,10-phenanthroline and 3-formylsalcylate anion; the apical site is occupied by the O atom of water. The 3-formylsalicylate anion acts as a bidentate ligand. The O atom of the formyl group is not coordinated.

There are three kinds of intermolecular hydrogen bonds in the crystal. One is between the H atom of water and the O atom of methanol, the second is between the H atom of water and the formyl O atom, the third is between the H atom of methanol and the uncoordinated O atom of the carboxylate group. The intermolecular hydrogen bonds link the molecules into a onedimensional chain, running in the [1 - 1 0] direction (Figure 2).

Experimental

3-formylsalicylic acid (0.166 g, 1.0 mmol) was dissolved in 10 ml NaOH (0.080 g, 2.0 mmol) aqueous solution. To this solution, 15 ml me thanol solution containing 1,10-phenanthroline (0.1982 g, 1 mmol) and $CuCl_2.2H_2O$ (0.1705 g, 1 mmol) was added. The mixture was stirred at ambient temperature for 2 h, then filtered to give a green solution. The filtrate was airproofed and kept at room temperature. Two weeks later, green block-shaped crystal of X-ray quality were obtained.

Refinement

The approximate positions of the water H atoms, obtained from a difference Fourier map, were restrained to ideal water geometry and fixed in the final stages of refinement. All other H atoms were included in calculated positions, with C—H distances ranging from 0.93 to 0.96 Å and O—H distances of 0.82 Å. They were refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C, O).

Figures

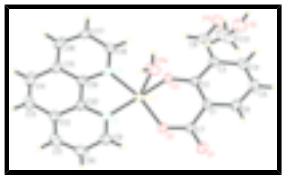

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

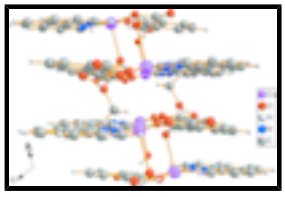

Fig. 2. The molecular packing of the title compound. Hydrogen bonds are indicated by dashed lines.

Aqua(3-formyl-2-oxidobenzoato-κ^2*O*^{1},*O*^{2})(1,10-phenanthroline- κ^2*N*,*N*')copper(II) methanol solvate

Crystal data

$[Cu(C_8H_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot CH_4O$	$Z = 2$
$M_r = 457.91$	$F_{000} = 470$
Triclinic, $P\overline{1}$	$D_x = 1.605$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.6714$ (11) Å	Cell parameters from 1476 reflections
$b = 10.3895$ (13) Å	$\theta = 2.4$–23.1°
$c = 11.7617$ (14) Å	$\mu = 1.20$ mm^{-1}
$\alpha = 115.125$ (2)°	$T = 296$ (2) K
$\beta = 95.859$ (2)°	Block, green
$\gamma = 93.589$ (2)°	0.21 × 0.16 × 0.15 mm
$V = 947.7$ (2) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	2336 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.061$
Monochromator: graphite	$\theta_{max} = 25.0^\circ$
$T = 296(2)$ K	$\theta_{min} = 1.9^\circ$
φ and ω scans	$h = -10\rightarrow8$
Absorption correction: none	$k = -11\rightarrow12$
4953 measured reflections	$l = -13\rightarrow11$
3336 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.100$

$S = 0.94$

3336 reflections

273 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.56$ e Å^{-3}

$\Delta\rho_{min} = -0.40$ e Å^{-3}

Extinction correction: none

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	0.04891 (5)	0.15042 (5)	0.43931 (4)	0.04238 (18)
O1W	0.2655 (3)	0.2918 (3)	0.4306 (3)	0.0690 (8)
H1WA	0.3370	0.2382	0.4054	0.083*
H1WB	0.2452	0.3275	0.3785	0.083*
N1	−0.1078 (3)	0.2009 (3)	0.3305 (3)	0.0395 (7)
N2	0.0517 (3)	−0.0202 (3)	0.2729 (3)	0.0366 (7)
O1	0.0334 (3)	0.4719 (2)	0.7766 (2)	0.0541 (7)
O2	−0.0072 (3)	0.3010 (3)	0.5848 (2)	0.0518 (7)
O3	0.1798 (3)	0.0801 (2)	0.5341 (2)	0.0433 (6)
O4	0.5232 (3)	−0.0845 (3)	0.6619 (3)	0.0694 (9)
C1	0.2080 (4)	0.2978 (3)	0.7301 (3)	0.0344 (8)
C2	0.2507 (4)	0.1602 (3)	0.6484 (3)	0.0347 (8)
C3	0.3754 (4)	0.1093 (4)	0.6985 (3)	0.0364 (8)
C4	0.4531 (4)	0.1902 (4)	0.8211 (4)	0.0455 (9)
H4A	0.5349	0.1545	0.8517	0.055*
C5	0.4121 (5)	0.3205 (4)	0.8972 (4)	0.0517 (10)
H5A	0.4649	0.3738	0.9788	0.062*
C6	0.2905 (4)	0.3714 (4)	0.8503 (3)	0.0433 (9)
H6A	0.2624	0.4601	0.9025	0.052*
C7	0.0722 (4)	0.3618 (4)	0.6951 (3)	0.0377 (8)
C8	0.4236 (4)	−0.0293 (4)	0.6237 (4)	0.0480 (10)
H8A	0.3748	−0.0798	0.5404	0.058*

C9	−0.1828 (4)	0.3141 (4)	0.3596 (4)	0.0511 (10)
H9A	−0.1596	0.3876	0.4413	0.061*
C10	−0.2942 (5)	0.3298 (4)	0.2752 (4)	0.0560 (11)
H10A	−0.3451	0.4116	0.3005	0.067*
C11	−0.3287 (5)	0.2251 (4)	0.1550 (4)	0.0554 (11)
H11A	−0.4043	0.2347	0.0979	0.066*
C12	−0.2512 (4)	0.1027 (4)	0.1166 (3)	0.0429 (9)
C13	−0.2754 (5)	−0.0140 (4)	−0.0074 (4)	0.0534 (11)
H13A	−0.3494	−0.0119	−0.0695	0.064*
C14	−0.1935 (5)	−0.1267 (4)	−0.0360 (4)	0.0546 (11)
H14A	−0.2120	−0.2007	−0.1177	0.066*
C15	−0.0787 (4)	−0.1356 (4)	0.0558 (3)	0.0421 (9)
C16	0.0130 (5)	−0.2480 (4)	0.0336 (3)	0.0505 (10)
H16A	0.0007	−0.3254	−0.0461	0.061*
C17	0.1192 (5)	−0.2437 (4)	0.1277 (4)	0.0493 (10)
H17A	0.1810	−0.3178	0.1126	0.059*
C18	0.1366 (4)	−0.1285 (4)	0.2479 (3)	0.0429 (9)
H18A	0.2095	−0.1276	0.3120	0.051*
C19	−0.0538 (4)	−0.0235 (4)	0.1789 (3)	0.0362 (8)
C20	−0.1402 (4)	0.0960 (4)	0.2081 (3)	0.0373 (8)
C21	0.6449 (6)	0.4308 (6)	0.6735 (6)	0.108 (2)
H21A	0.6025	0.4468	0.7501	0.162*
H21B	0.6887	0.3416	0.6434	0.162*
H21C	0.5635	0.4275	0.6103	0.162*
O5	0.7606 (4)	0.5414 (3)	0.6979 (3)	0.0751 (9)
H5	0.8459	0.5183	0.7138	0.113*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0434 (3)	0.0424 (3)	0.0300 (3)	0.0188 (2)	0.00278 (19)	0.0037 (2)
O1W	0.0605 (19)	0.0671 (19)	0.092 (2)	0.0250 (16)	0.0175 (17)	0.0422 (18)
N1	0.0402 (18)	0.0358 (17)	0.0363 (17)	0.0096 (15)	0.0087 (14)	0.0085 (14)
N2	0.0324 (17)	0.0363 (17)	0.0342 (17)	0.0068 (14)	0.0089 (14)	0.0074 (14)
O1	0.0666 (19)	0.0384 (15)	0.0413 (15)	0.0236 (14)	0.0049 (14)	0.0001 (13)
O2	0.0540 (17)	0.0520 (16)	0.0321 (14)	0.0283 (14)	0.0016 (12)	0.0000 (12)
O3	0.0487 (16)	0.0346 (13)	0.0327 (14)	0.0154 (12)	−0.0007 (12)	0.0014 (11)
O4	0.0579 (19)	0.0649 (19)	0.092 (2)	0.0275 (16)	0.0107 (17)	0.0382 (18)
C1	0.036 (2)	0.0324 (19)	0.0313 (19)	0.0047 (16)	0.0042 (16)	0.0100 (16)
C2	0.034 (2)	0.036 (2)	0.034 (2)	0.0034 (17)	0.0070 (16)	0.0144 (17)
C3	0.032 (2)	0.037 (2)	0.042 (2)	0.0041 (17)	0.0067 (17)	0.0188 (18)
C4	0.036 (2)	0.051 (2)	0.055 (3)	0.0044 (19)	0.0007 (19)	0.030 (2)
C5	0.054 (3)	0.049 (2)	0.042 (2)	−0.003 (2)	−0.012 (2)	0.015 (2)
C6	0.050 (2)	0.033 (2)	0.037 (2)	0.0011 (18)	0.0020 (18)	0.0064 (17)
C7	0.041 (2)	0.034 (2)	0.032 (2)	0.0050 (17)	0.0070 (17)	0.0079 (17)
C8	0.041 (2)	0.049 (2)	0.057 (3)	0.011 (2)	0.012 (2)	0.024 (2)
C9	0.049 (2)	0.046 (2)	0.055 (3)	0.014 (2)	0.009 (2)	0.018 (2)
C10	0.050 (3)	0.054 (3)	0.068 (3)	0.019 (2)	0.008 (2)	0.029 (2)

C11	0.051 (3)	0.064 (3)	0.060 (3)	0.006 (2)	−0.003 (2)	0.038 (3)
C12	0.039 (2)	0.050 (2)	0.042 (2)	−0.0015 (19)	0.0021 (18)	0.025 (2)
C13	0.057 (3)	0.062 (3)	0.041 (2)	−0.011 (2)	−0.009 (2)	0.029 (2)
C14	0.066 (3)	0.053 (3)	0.033 (2)	−0.012 (2)	−0.001 (2)	0.010 (2)
C15	0.044 (2)	0.042 (2)	0.033 (2)	−0.0061 (19)	0.0078 (18)	0.0098 (17)
C16	0.058 (3)	0.042 (2)	0.034 (2)	−0.003 (2)	0.016 (2)	−0.0004 (19)
C17	0.054 (3)	0.036 (2)	0.048 (2)	0.0128 (19)	0.022 (2)	0.0048 (19)
C18	0.037 (2)	0.043 (2)	0.044 (2)	0.0078 (18)	0.0091 (18)	0.0141 (18)
C19	0.037 (2)	0.038 (2)	0.0274 (19)	−0.0022 (17)	0.0053 (16)	0.0089 (16)
C20	0.035 (2)	0.043 (2)	0.032 (2)	−0.0003 (18)	0.0048 (17)	0.0157 (18)
C21	0.068 (4)	0.116 (5)	0.173 (6)	0.040 (4)	0.040 (4)	0.085 (5)
O5	0.078 (2)	0.0586 (19)	0.085 (2)	0.0297 (18)	0.001 (2)	0.0276 (18)

Geometric parameters (Å, °)

Cu1—O1W	2.348 (3)	C8—H8A	0.9300
Cu1—O2	1.898 (2)	C9—C10	1.381 (5)
Cu1—O3	1.898 (2)	C9—H9A	0.9300
Cu1—N1	2.016 (3)	C10—C11	1.356 (5)
Cu1—N2	2.011 (3)	C10—H10A	0.9300
O1W—H1WA	0.8500	C11—C12	1.399 (5)
O1W—H1WB	0.8499	C11—H11A	0.9300
N1—C9	1.312 (4)	C12—C20	1.396 (5)
N1—C20	1.373 (4)	C12—C13	1.430 (5)
N2—C18	1.327 (4)	C13—C14	1.344 (5)
N2—C19	1.348 (4)	C13—H13A	0.9300
O1—C7	1.234 (4)	C14—C15	1.430 (5)
O2—C7	1.273 (4)	C14—H14A	0.9300
O3—C2	1.301 (4)	C15—C16	1.401 (5)
O4—C8	1.216 (4)	C15—C19	1.403 (4)
C1—C6	1.380 (5)	C16—C17	1.350 (5)
C1—C2	1.441 (4)	C16—H16A	0.9300
C1—C7	1.494 (5)	C17—C18	1.397 (5)
C2—C3	1.415 (5)	C17—H17A	0.9300
C3—C4	1.394 (5)	C18—H18A	0.9300
C3—C8	1.448 (5)	C19—C20	1.424 (5)
C4—C5	1.363 (5)	C21—O5	1.388 (5)
C4—H4A	0.9300	C21—H21A	0.9600
C5—C6	1.375 (5)	C21—H21B	0.9600
C5—H5A	0.9300	C21—H21C	0.9600
C6—H6A	0.9300	O5—H5	0.8200
O1W—Cu1—O2	93.40 (11)	C3—C8—H8A	117.6
O1W—Cu1—O3	90.04 (10)	N1—C9—C10	123.4 (4)
O1W—Cu1—N1	96.50 (11)	N1—C9—H9A	118.3
O1W—Cu1—N2	97.69 (10)	C10—C9—H9A	118.3
O2—Cu1—O3	94.32 (10)	C11—C10—C9	119.5 (4)
O2—Cu1—N1	88.77 (11)	C11—C10—H10A	120.2
O2—Cu1—N2	166.01 (11)	C9—C10—H10A	120.2
O3—Cu1—N1	172.59 (11)	C10—C11—C12	120.2 (4)

O3—Cu1—N2	94.17 (11)	C10—C11—H11A	119.9
N1—Cu1—N2	81.55 (11)	C12—C11—H11A	119.9
Cu1—O1W—H1WA	107.8	C20—C12—C11	116.4 (4)
Cu1—O1W—H1WB	112.5	C20—C12—C13	118.0 (4)
H1WA—O1W—H1WB	107.7	C11—C12—C13	125.6 (4)
C9—N1—C20	117.2 (3)	C14—C13—C12	121.4 (4)
C9—N1—Cu1	130.2 (3)	C14—C13—H13A	119.3
C20—N1—Cu1	112.5 (2)	C12—C13—H13A	119.3
C18—N2—C19	118.4 (3)	C13—C14—C15	121.6 (4)
C18—N2—Cu1	128.5 (3)	C13—C14—H14A	119.2
C19—N2—Cu1	113.0 (2)	C15—C14—H14A	119.2
C7—O2—Cu1	126.8 (2)	C16—C15—C19	116.4 (4)
C2—O3—Cu1	123.3 (2)	C16—C15—C14	125.3 (4)
C6—C1—C2	118.7 (3)	C19—C15—C14	118.3 (4)
C6—C1—C7	117.6 (3)	C17—C16—C15	120.0 (3)
C2—C1—C7	123.6 (3)	C17—C16—H16A	120.0
O3—C2—C3	118.8 (3)	C15—C16—H16A	120.0
O3—C2—C1	124.2 (3)	C16—C17—C18	120.2 (4)
C3—C2—C1	117.0 (3)	C16—C17—H17A	119.9
C4—C3—C2	120.9 (3)	C18—C17—H17A	119.9
C4—C3—C8	118.5 (3)	N2—C18—C17	121.7 (4)
C2—C3—C8	120.6 (3)	N2—C18—H18A	119.2
C5—C4—C3	121.6 (3)	C17—C18—H18A	119.2
C5—C4—H4A	119.2	N2—C19—C15	123.5 (3)
C3—C4—H4A	119.2	N2—C19—C20	116.9 (3)
C4—C5—C6	118.3 (4)	C15—C19—C20	119.6 (3)
C4—C5—H5A	120.8	N1—C20—C12	123.3 (3)
C6—C5—H5A	120.8	N1—C20—C19	115.7 (3)
C5—C6—C1	123.6 (3)	C12—C20—C19	121.0 (3)
C5—C6—H6A	118.2	O5—C21—H21A	109.5
C1—C6—H6A	118.2	O5—C21—H21B	109.5
O1—C7—O2	120.1 (3)	H21A—C21—H21B	109.5
O1—C7—C1	118.9 (3)	O5—C21—H21C	109.5
O2—C7—C1	120.9 (3)	H21A—C21—H21C	109.5
O4—C8—C3	124.8 (4)	H21B—C21—H21C	109.5
O4—C8—H8A	117.6	C21—O5—H5	109.5
O2—Cu1—N1—C9	12.7 (3)	C6—C1—C7—O2	178.7 (3)
N2—Cu1—N1—C9	−177.4 (3)	C2—C1—C7—O2	−5.4 (5)
O1W—Cu1—N1—C9	−80.5 (3)	C4—C3—C8—O4	3.6 (5)
O2—Cu1—N1—C20	−165.8 (2)	C2—C3—C8—O4	−175.6 (3)
N2—Cu1—N1—C20	4.1 (2)	C20—N1—C9—C10	2.1 (5)
O1W—Cu1—N1—C20	100.9 (2)	Cu1—N1—C9—C10	−176.3 (3)
O2—Cu1—N2—C18	−134.6 (4)	N1—C9—C10—C11	−0.8 (6)
O3—Cu1—N2—C18	−7.3 (3)	C9—C10—C11—C12	−0.5 (6)
N1—Cu1—N2—C18	178.7 (3)	C10—C11—C12—C20	0.4 (5)
O1W—Cu1—N2—C18	83.3 (3)	C10—C11—C12—C13	−179.2 (4)
O2—Cu1—N2—C19	42.0 (6)	C20—C12—C13—C14	−0.5 (5)
O3—Cu1—N2—C19	169.2 (2)	C11—C12—C13—C14	179.1 (4)
N1—Cu1—N2—C19	−4.7 (2)	C12—C13—C14—C15	0.2 (6)

O1W—Cu1—N2—C19	−100.2 (2)	C13—C14—C15—C16	−179.2 (3)
O3—Cu1—O2—C7	25.9 (3)	C13—C14—C15—C19	0.7 (5)
N2—Cu1—O2—C7	153.2 (4)	C19—C15—C16—C17	−0.6 (5)
N1—Cu1—O2—C7	−160.8 (3)	C14—C15—C16—C17	179.3 (3)
O1W—Cu1—O2—C7	−64.4 (3)	C15—C16—C17—C18	0.8 (6)
O2—Cu1—O3—C2	−27.2 (3)	C19—N2—C18—C17	0.2 (5)
N2—Cu1—O3—C2	163.9 (3)	Cu1—N2—C18—C17	176.6 (2)
O1W—Cu1—O3—C2	66.2 (3)	C16—C17—C18—N2	−0.7 (5)
Cu1—O3—C2—C3	−163.8 (2)	C18—N2—C19—C15	0.0 (5)
Cu1—O3—C2—C1	17.9 (4)	Cu1—N2—C19—C15	−176.9 (2)
C6—C1—C2—O3	178.8 (3)	C18—N2—C19—C20	−178.5 (3)
C7—C1—C2—O3	2.8 (5)	Cu1—N2—C19—C20	4.6 (4)
C6—C1—C2—C3	0.4 (5)	C16—C15—C19—N2	0.2 (5)
C7—C1—C2—C3	−175.5 (3)	C14—C15—C19—N2	−179.7 (3)
O3—C2—C3—C4	−178.9 (3)	C16—C15—C19—C20	178.6 (3)
C1—C2—C3—C4	−0.5 (5)	C14—C15—C19—C20	−1.2 (5)
O3—C2—C3—C8	0.3 (5)	C9—N1—C20—C12	−2.3 (5)
C1—C2—C3—C8	178.7 (3)	Cu1—N1—C20—C12	176.5 (3)
C2—C3—C4—C5	0.2 (5)	C9—N1—C20—C19	178.4 (3)
C8—C3—C4—C5	−179.0 (3)	Cu1—N1—C20—C19	−2.9 (4)
C3—C4—C5—C6	0.2 (5)	C11—C12—C20—N1	1.1 (5)
C4—C5—C6—C1	−0.3 (6)	C13—C12—C20—N1	−179.4 (3)
C2—C1—C6—C5	−0.1 (5)	C11—C12—C20—C19	−179.7 (3)
C7—C1—C6—C5	176.1 (3)	C13—C12—C20—C19	−0.1 (5)
Cu1—O2—C7—O1	169.4 (2)	N2—C19—C20—N1	−1.1 (4)
Cu1—O2—C7—C1	−13.8 (5)	C15—C19—C20—N1	−179.7 (3)
C6—C1—C7—O1	−4.5 (5)	N2—C19—C20—C12	179.5 (3)
C2—C1—C7—O1	171.4 (3)	C15—C19—C20—C12	0.9 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O1^{i}	0.82	1.89	2.703 (4)	171
O1W—H1WB···O5^{ii}	0.85	1.93	2.747 (4)	162
O1W—H1WA···O4^{iii}	0.85	2.00	2.844 (4)	170

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

Fig. 1

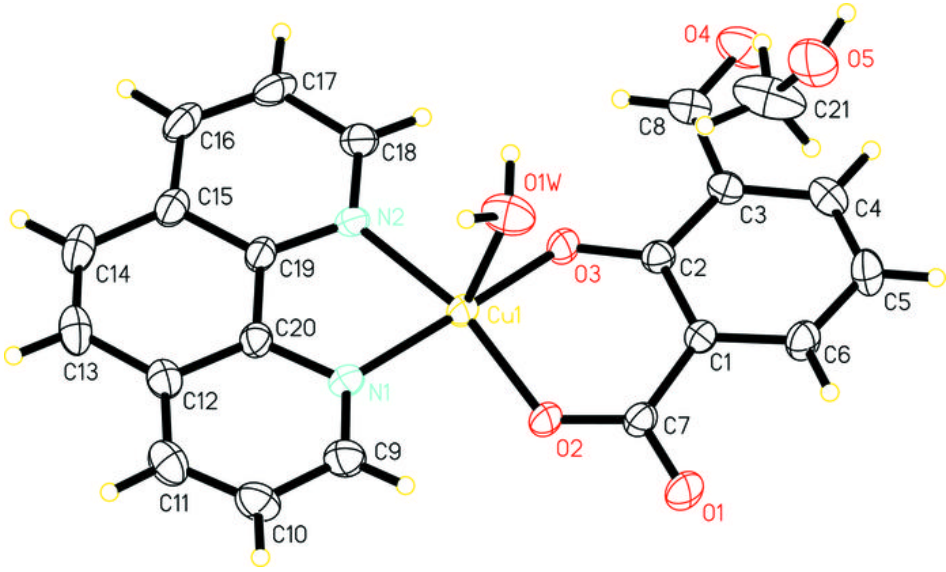
C17
C16
C18
C15
N2
C14
C19
C20
C13
C12
N1
C9
C11
C10
O1W
Cu1
O3
O2
C2
C1
C7
O1
C8
O4
O5
C21
C3
C4
C5
C6

Fig. 2