Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(4-formylbenzoato-κO)(nitrato-κO)-(1,10-phenanthroline-$\kappa^2 N,N'$)copper(II)

Zhao-Peng Deng, Shan Gao,* Li-Hua Huo and Hui Zhao

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: shangao67@yahoo.com

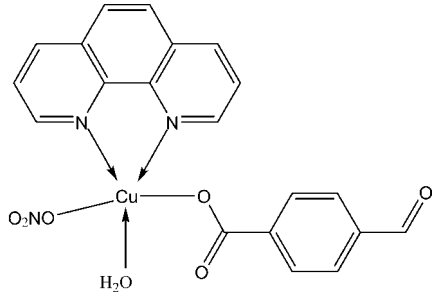
Received 9 October 2007; accepted 10 October 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.157; data-to-parameter ratio = 14.8.

In the title complex, $[Cu(C_8H_5O_3)(NO_3)(C_{12}H_8N_2)(H_2O)]$, the Cu^{II} atom adopts a distorted square-pyramidal coordination geometry with an O atom of the nitrate group occupying the apex of the pyramid. The complex molecules are linked into ribbons along the *a* axis *via* hydrogen bonding between the water molecule and the nitro anion. π–π stacking interactions between the 4-formylbenzoate and phenanthroline ligands assemble two ribbons into a larger one-dimensional structure. The centroid-to-centroid distances between the overlapping six-membered rings are 3.634 (3) and 3.722 (3) Å.

Related literature

For literature on copper 4-formylbenzoate complexes, see: Deng *et al.* (2006).



Experimental

Crystal data

$[Cu(C_8H_5O_3)(NO_3)(C_{12}H_8N_2)(H_2O)]$
M_r = 472.89
Triclinic, $P\overline{1}$
a = 7.6070 (15) Å
b = 9.0859 (18) Å
c = 14.147 (3) Å
α = 88.88 (3)°
β = 74.49 (3)°
γ = 86.60 (3)°
V = 940.5 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.21 mm^{-1}
T = 295 (2) K
0.32 × 0.25 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.699, T_{max} = 0.807
9201 measured reflections
4247 independent reflections
2405 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.157
S = 1.09
4247 reflections
286 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.947 (3)	Cu1—N1	2.004 (3)
Cu1—O1W	1.965 (3)	Cu1—O4	2.337 (3)
Cu1—N2	2.002 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2	0.85 (3)	1.696 (15)	2.520 (5)	164 (5)
O1W—H1W2···O6^{i}	0.85 (3)	1.870 (12)	2.714 (4)	175 (5)

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the Heilongjiang Province Natural Science Foundation (grant No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (grant No. 1054 G036) and Heilongjiang University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2110).

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 doi:10.1107/S1600536807049744

supplementary materials

Acta Cryst. (2007). E**63**, m2739 [**doi:10.1107/S1600536807049744**]

Aqua(4-formylbenzoato-κO)(nitrato-κO)(1,10-phenanthroline-$\kappa^2 N,N'$)copper(II)

Z.-P. Deng, S. Gao, L.-H. Huo and H. Zhao

Comment

In our previous work, we have reported the synthesis and structure of complex $[Cu(C_8H_5O_3)_2(H_2O)_2]\cdot 2H_2O$, (I) (Deng *et al.*, 2006), which can be obtained by the reaction of $Cu(X)_2$ (X = Ac, NO_3, Cl) and 4-formylbenzoic acid in a aqueous solution. We have noticed that in the presence of 4-formylbenzoic acid the anion X was not coordinating to the copper(II) atom. But for the title complex, we introduced the 1,10-phenanthroline ligand to the system of $Cu(NO_3)_2$ and 4-formylbenzoic acid in a H_2O/EtOH solution, and obtained a new complex $[Cu(NO_3)(C_8H_5O_3)(C_{12}H_8N_2)(H_2O)]$, (II), in which the copper(II) atom is five-coordinated by nitrate group and formylbenzoate carboxylate group in monodentate mode, 1.10-phenanthroline ligand in chelating mode as well as a water molecule (Fig.1). Adjacent complex molecules are linked into a one-dimensional chain structure *via* hydrogen-bonding interactions and π-π stacking interactions between the benzene rings of phenanthroline and 4-formylbenzoato ligand, with centroid-centroid distances of 3.634 (3) (*Cg*1 and *Cg*2) and 3.722 (3) Å (*Cg*2 and *Cg*3) [*Cg*1: C15^{i}—C18^{i}/N2^{i}/C19^{i}; *Cg*2: C2^{ii}—C7^{ii}; *Cg*3: C12—C15/C19—C20, symmetry code: (I) $x-1,y,z$; (II) $-x+1,-y+1,-z+1$; Fig.2].

Experimental

Copper(II) nitrate hexahydrate (1.48 g, 5 mmol) was added to a H_2O/EtOH solution (1:1 *v*/*v*) of 4-formylbenzoic acid (1.5 g, 10 mmol) and 1,10-phenanthroline (0.99 g 5 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until pH = 5 was reached. Blue single crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{20}H_{15}N_3O_7Cu$: C 50.80, H 3.20, N 8.89. Found: C 50.85, H 3.24, N 8.82.

Refinement

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 and $U_{iso}(H) = 1.2U_{eq}$ (C), and were included in the refinement in the riding model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with the O—H and H···H distance restraints to 0.85 (1) and 1.39 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

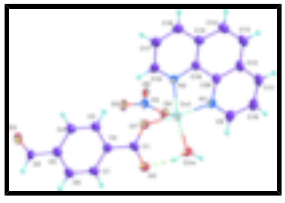

Fig. 1. Molecular structure of the title compound with 30% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

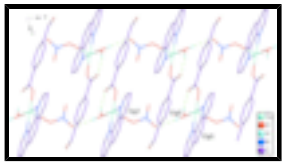

Fig. 2. one-dimensional-chain structure of the title complex along the *a* axis formed by hydrogen-bonding and π-π stacking interactions, with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted. *Cg*1, *Cg*2 and *Cg*3 represent the centroids of adjacent benzene rings of phen ligands and 4-formylbenzoato ligand, as defined in the Comment.

Aqua(4-formylbenzoato-κ*O*)(nitrato-κ*O*)(1,10-phenanthroline- κ^2N,N')copper(II)

Crystal data

$[Cu(C_8H_5O_3)(NO_3)(C_{12}H_8N_2)(H_2O)]$	$Z = 2$
$M_r = 472.89$	$F_{000} = 482$
Triclinic, $P\overline{1}$	$D_x = 1.670$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.6070$ (15) Å	Cell parameters from 4431 reflections
$b = 9.0859$ (18) Å	$\theta = 3.5$–27.4º
$c = 14.147$ (3) Å	$\mu = 1.21$ mm^{-1}
$\alpha = 88.88$ (3)º	$T = 295$ (2) K
$\beta = 74.49$ (3)º	Prism, blue
$\gamma = 86.60$ (3)º	0.32 × 0.25 × 0.18 mm
$V = 940.5$ (4) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4247 independent reflections
Radiation source: fine-focus sealed tube	2405 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.4$º
$T = 295(2)$ K	$\theta_{min} = 3.5$º
ω scans	$h = -9 \rightarrow 7$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11 \rightarrow 11$
$T_{min} = 0.699$, $T_{max} = 0.807$	$l = -18 \rightarrow 18$
9201 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.157$	$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$

4247 reflections	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
286 parameters	$\Delta\rho_{min}$ = −0.68 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.54659 (7)	0.45156 (5)	0.68949 (4)	0.0463 (2)
O1W	0.3833 (4)	0.2877 (3)	0.7229 (2)	0.0532 (7)
H1W1	0.411 (5)	0.242 (5)	0.6689 (19)	0.080*
H1W2	0.2684 (17)	0.300 (5)	0.745 (3)	0.080*
O1	0.6488 (4)	0.3948 (3)	0.5529 (2)	0.0536 (7)
O2	0.5177 (5)	0.1807 (4)	0.5543 (3)	0.0758 (10)
O3	1.1474 (6)	0.2219 (5)	0.0636 (3)	0.0959 (13)
O4	0.7526 (4)	0.3261 (4)	0.7633 (2)	0.0685 (10)
O5	0.9981 (5)	0.2915 (5)	0.6474 (3)	0.0885 (12)
O6	1.0143 (4)	0.3075 (4)	0.7949 (2)	0.0653 (9)
N1	0.4366 (4)	0.5431 (4)	0.8214 (2)	0.0470 (8)
N2	0.6552 (4)	0.6481 (4)	0.6598 (2)	0.0429 (8)
N3	0.9214 (5)	0.3087 (4)	0.7339 (3)	0.0462 (8)
C1	0.6249 (6)	0.2757 (4)	0.5128 (3)	0.0484 (10)
C2	0.7352 (5)	0.2457 (4)	0.4095 (3)	0.0461 (10)
C3	0.8376 (6)	0.3544 (5)	0.3519 (3)	0.0489 (10)
H3	0.8364	0.4483	0.3771	0.059*
C4	0.9389 (6)	0.3223 (5)	0.2587 (3)	0.0527 (11)
H4	1.0070	0.3947	0.2209	0.063*
C5	0.9418 (6)	0.1814 (5)	0.2190 (3)	0.0514 (10)
C6	0.8392 (6)	0.0743 (5)	0.2771 (3)	0.0537 (11)
H6	0.8400	−0.0197	0.2520	0.064*
C7	0.7369 (6)	0.1062 (4)	0.3709 (3)	0.0512 (10)
H7	0.6685	0.0341	0.4088	0.061*
C8	1.0505 (7)	0.1427 (6)	0.1195 (4)	0.0686 (14)
H8	1.0431	0.0476	0.0982	0.082*
C9	0.3303 (6)	0.4855 (5)	0.9034 (3)	0.0581 (12)
H9	0.3038	0.3869	0.9036	0.070*
C10	0.2590 (7)	0.5672 (6)	0.9875 (3)	0.0668 (13)
H10	0.1885	0.5226	1.0434	0.080*
C11	0.2912 (7)	0.7120 (6)	0.9890 (3)	0.0641 (13)
H11	0.2408	0.7670	1.0455	0.077*
C12	0.4011 (6)	0.7796 (5)	0.9049 (3)	0.0507 (11)
C13	0.4415 (6)	0.9304 (5)	0.8971 (4)	0.0589 (12)
H13	0.3901	0.9930	0.9496	0.071*
C14	0.5541 (6)	0.9851 (5)	0.8140 (4)	0.0574 (12)
H14	0.5790	1.0844	0.8110	0.069*
C15	0.6352 (6)	0.8924 (5)	0.7309 (3)	0.0487 (10)
C16	0.7539 (6)	0.9401 (5)	0.6428 (3)	0.0553 (11)

H16	0.7877	1.0373	0.6359	0.066*
C17	0.8188 (6)	0.8433 (5)	0.5681 (3)	0.0576 (11)
H17	0.8985	0.8737	0.5100	0.069*
C18	0.7654 (6)	0.6971 (5)	0.5787 (3)	0.0529 (11)
H18	0.8096	0.6327	0.5263	0.063*
C19	0.5920 (5)	0.7451 (4)	0.7358 (3)	0.0440 (9)
C20	0.4725 (5)	0.6878 (4)	0.8236 (3)	0.0449 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0447 (3)	0.0530 (3)	0.0389 (3)	−0.0098 (2)	−0.0057 (2)	−0.0038 (2)
O1W	0.0412 (16)	0.0584 (18)	0.055 (2)	−0.0149 (13)	−0.0018 (14)	−0.0017 (14)
O1	0.0620 (19)	0.0583 (17)	0.0393 (17)	−0.0189 (14)	−0.0075 (14)	−0.0080 (13)
O2	0.078 (2)	0.065 (2)	0.070 (2)	−0.0312 (17)	0.0103 (19)	−0.0187 (17)
O3	0.101 (3)	0.104 (3)	0.065 (3)	0.008 (2)	0.005 (2)	0.003 (2)
O4	0.0388 (18)	0.103 (3)	0.059 (2)	0.0005 (16)	−0.0078 (16)	0.0154 (18)
O5	0.075 (3)	0.137 (3)	0.043 (2)	−0.007 (2)	0.0047 (19)	−0.018 (2)
O6	0.0442 (18)	0.099 (2)	0.051 (2)	−0.0018 (16)	−0.0079 (16)	−0.0120 (17)
N1	0.0404 (19)	0.055 (2)	0.043 (2)	−0.0061 (15)	−0.0053 (16)	−0.0023 (16)
N2	0.0417 (19)	0.0525 (19)	0.0313 (18)	−0.0106 (14)	−0.0024 (15)	−0.0031 (14)
N3	0.042 (2)	0.0527 (19)	0.040 (2)	−0.0091 (15)	−0.0017 (17)	−0.0012 (15)
C1	0.052 (3)	0.048 (2)	0.046 (3)	−0.0050 (18)	−0.014 (2)	−0.0095 (19)
C2	0.042 (2)	0.056 (2)	0.042 (2)	−0.0051 (18)	−0.0116 (19)	−0.0055 (19)
C3	0.055 (3)	0.050 (2)	0.042 (3)	−0.0082 (19)	−0.012 (2)	−0.0044 (18)
C4	0.058 (3)	0.050 (2)	0.049 (3)	−0.0087 (19)	−0.012 (2)	−0.001 (2)
C5	0.050 (3)	0.057 (2)	0.047 (3)	−0.0014 (19)	−0.014 (2)	−0.006 (2)
C6	0.056 (3)	0.055 (2)	0.050 (3)	−0.004 (2)	−0.012 (2)	−0.015 (2)
C7	0.051 (3)	0.049 (2)	0.055 (3)	−0.0085 (18)	−0.014 (2)	−0.009 (2)
C8	0.063 (3)	0.084 (4)	0.053 (3)	0.001 (3)	−0.007 (3)	0.001 (3)
C9	0.057 (3)	0.071 (3)	0.042 (3)	−0.010 (2)	−0.003 (2)	0.004 (2)
C10	0.066 (3)	0.083 (4)	0.039 (3)	−0.010 (3)	0.008 (2)	0.001 (2)
C11	0.059 (3)	0.085 (4)	0.041 (3)	0.003 (2)	−0.001 (2)	−0.019 (2)
C12	0.050 (3)	0.066 (3)	0.036 (2)	0.005 (2)	−0.011 (2)	−0.013 (2)
C13	0.066 (3)	0.061 (3)	0.053 (3)	0.006 (2)	−0.021 (2)	−0.020 (2)
C14	0.063 (3)	0.054 (2)	0.062 (3)	0.000 (2)	−0.028 (3)	−0.012 (2)
C15	0.048 (3)	0.055 (2)	0.047 (3)	−0.0047 (19)	−0.020 (2)	−0.005 (2)
C16	0.063 (3)	0.054 (2)	0.052 (3)	−0.019 (2)	−0.018 (2)	0.003 (2)
C17	0.064 (3)	0.066 (3)	0.043 (3)	−0.020 (2)	−0.011 (2)	−0.002 (2)
C18	0.051 (3)	0.070 (3)	0.036 (2)	−0.018 (2)	−0.004 (2)	−0.004 (2)
C19	0.042 (2)	0.056 (2)	0.035 (2)	−0.0035 (17)	−0.0119 (18)	−0.0058 (18)
C20	0.041 (2)	0.052 (2)	0.042 (2)	0.0027 (18)	−0.0132 (19)	−0.0045 (19)

Geometric parameters (Å, °)

Cu1—O1	1.947 (3)	C5—C8	1.467 (6)
Cu1—O1W	1.965 (3)	C6—C7	1.374 (6)
Cu1—N2	2.002 (3)	C6—H6	0.9300
Cu1—N1	2.004 (3)	C7—H7	0.9300

Cu1—O4	2.337 (3)	C8—H8	0.9300
O1W—H1W1	0.85 (3)	C9—C10	1.379 (7)
O1W—H1W2	0.85 (3)	C9—H9	0.9300
O1—C1	1.276 (5)	C10—C11	1.354 (7)
O2—C1	1.250 (5)	C10—H10	0.9300
O3—C8	1.190 (6)	C11—C12	1.411 (6)
O4—N3	1.241 (4)	C11—H11	0.9300
O5—N3	1.215 (4)	C12—C20	1.401 (6)
O6—N3	1.252 (4)	C12—C13	1.418 (6)
N1—C9	1.341 (5)	C13—C14	1.360 (7)
N1—C20	1.362 (5)	C13—H13	0.9300
N2—C18	1.314 (5)	C14—C15	1.436 (6)
N2—C19	1.370 (5)	C14—H14	0.9300
C1—C2	1.499 (6)	C15—C19	1.392 (6)
C2—C7	1.388 (6)	C15—C16	1.407 (6)
C2—C3	1.403 (6)	C16—C17	1.357 (6)
C3—C4	1.365 (6)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.406 (6)
C4—C5	1.405 (6)	C17—H17	0.9300
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.396 (6)	C19—C20	1.438 (6)
O1—Cu1—O1W	95.24 (13)	C6—C7—C2	120.3 (4)
O1—Cu1—N2	89.81 (13)	C6—C7—H7	119.9
O1W—Cu1—N2	165.89 (13)	C2—C7—H7	119.9
O1—Cu1—N1	170.66 (12)	O3—C8—C5	125.9 (5)
O1W—Cu1—N1	91.10 (13)	O3—C8—H8	117.1
N2—Cu1—N1	82.47 (13)	C5—C8—H8	117.1
O1—Cu1—O4	101.06 (13)	N1—C9—C10	122.4 (5)
O1W—Cu1—O4	90.02 (12)	N1—C9—H9	118.8
N2—Cu1—O4	101.96 (13)	C10—C9—H9	118.8
N1—Cu1—O4	85.75 (13)	C11—C10—C9	120.4 (5)
Cu1—O1W—H1W1	101 (3)	C11—C10—H10	119.8
Cu1—O1W—H1W2	123 (3)	C9—C10—H10	119.8
H1W1—O1W—H1W2	111 (4)	C10—C11—C12	120.1 (4)
C1—O1—Cu1	126.9 (3)	C10—C11—H11	120.0
N3—O4—Cu1	129.6 (3)	C12—C11—H11	120.0
C9—N1—C20	117.3 (4)	C20—C12—C11	115.9 (4)
C9—N1—Cu1	130.1 (3)	C20—C12—C13	118.9 (4)
C20—N1—Cu1	112.6 (3)	C11—C12—C13	125.2 (4)
C18—N2—C19	117.6 (4)	C14—C13—C12	121.2 (4)
C18—N2—Cu1	129.9 (3)	C14—C13—H13	119.4
C19—N2—Cu1	112.3 (3)	C12—C13—H13	119.4
O5—N3—O4	121.4 (4)	C13—C14—C15	121.1 (4)
O5—N3—O6	119.4 (4)	C13—C14—H14	119.4
O4—N3—O6	119.2 (4)	C15—C14—H14	119.4
O2—C1—O1	124.5 (4)	C19—C15—C16	116.8 (4)
O2—C1—C2	117.5 (4)	C19—C15—C14	118.6 (4)
O1—C1—C2	118.0 (4)	C16—C15—C14	124.6 (4)
C7—C2—C3	119.6 (4)	C17—C16—C15	119.5 (4)

C7—C2—C1	118.8 (4)	C17—C16—H16	120.3
C3—C2—C1	121.6 (4)	C15—C16—H16	120.3
C4—C3—C2	119.9 (4)	C16—C17—C18	120.0 (4)
C4—C3—H3	120.0	C16—C17—H17	120.0
C2—C3—H3	120.0	C18—C17—H17	120.0
C3—C4—C5	120.9 (4)	N2—C18—C17	122.4 (4)
C3—C4—H4	119.5	N2—C18—H18	118.8
C5—C4—H4	119.5	C17—C18—H18	118.8
C6—C5—C4	118.5 (4)	N2—C19—C15	123.7 (4)
C6—C5—C8	119.1 (4)	N2—C19—C20	116.2 (4)
C4—C5—C8	122.4 (4)	C15—C19—C20	120.1 (4)
C7—C6—C5	120.7 (4)	N1—C20—C12	123.9 (4)
C7—C6—H6	119.6	N1—C20—C19	116.0 (4)
C5—C6—H6	119.6	C12—C20—C19	120.1 (4)
O1W—Cu1—O1—C1	−8.8 (4)	C6—C5—C8—O3	−177.9 (5)
N2—Cu1—O1—C1	−175.6 (4)	C4—C5—C8—O3	1.3 (8)
O4—Cu1—O1—C1	82.3 (4)	C20—N1—C9—C10	−0.1 (6)
O1—Cu1—O4—N3	40.4 (4)	Cu1—N1—C9—C10	−177.0 (3)
O1W—Cu1—O4—N3	135.8 (4)	N1—C9—C10—C11	1.6 (8)
N2—Cu1—O4—N3	−51.8 (4)	C9—C10—C11—C12	−1.2 (8)
N1—Cu1—O4—N3	−133.1 (4)	C10—C11—C12—C20	−0.6 (7)
O1W—Cu1—N1—C9	15.0 (4)	C10—C11—C12—C13	178.8 (4)
N2—Cu1—N1—C9	−177.6 (4)	C20—C12—C13—C14	−2.9 (6)
O4—Cu1—N1—C9	−74.9 (4)	C11—C12—C13—C14	177.7 (4)
O1W—Cu1—N1—C20	−162.0 (3)	C12—C13—C14—C15	0.4 (7)
N2—Cu1—N1—C20	5.4 (3)	C13—C14—C15—C19	1.8 (6)
O4—Cu1—N1—C20	108.1 (3)	C13—C14—C15—C16	−179.5 (4)
O1—Cu1—N2—C18	−6.0 (4)	C19—C15—C16—C17	0.4 (6)
O1W—Cu1—N2—C18	−117.2 (6)	C14—C15—C16—C17	−178.3 (4)
N1—Cu1—N2—C18	179.3 (4)	C15—C16—C17—C18	0.8 (7)
O4—Cu1—N2—C18	95.3 (4)	C19—N2—C18—C17	0.0 (6)
O1—Cu1—N2—C19	169.6 (3)	Cu1—N2—C18—C17	175.3 (3)
O1W—Cu1—N2—C19	58.4 (6)	C16—C17—C18—N2	−1.0 (7)
N1—Cu1—N2—C19	−5.2 (3)	C18—N2—C19—C15	1.3 (6)
O4—Cu1—N2—C19	−89.2 (3)	Cu1—N2—C19—C15	−174.8 (3)
Cu1—O4—N3—O5	−36.2 (6)	C18—N2—C19—C20	−179.7 (4)
Cu1—O4—N3—O6	144.4 (3)	Cu1—N2—C19—C20	4.1 (4)
Cu1—O1—C1—O2	6.3 (7)	C16—C15—C19—N2	−1.5 (6)
Cu1—O1—C1—C2	−172.4 (2)	C14—C15—C19—N2	177.3 (4)
O2—C1—C2—C7	−10.6 (6)	C16—C15—C19—C20	179.6 (4)
O1—C1—C2—C7	168.3 (4)	C14—C15—C19—C20	−1.6 (6)
O2—C1—C2—C3	170.1 (4)	C9—N1—C20—C12	−1.9 (6)
O1—C1—C2—C3	−11.1 (6)	Cu1—N1—C20—C12	175.5 (3)
C7—C2—C3—C4	−0.5 (6)	C9—N1—C20—C19	177.8 (4)
C1—C2—C3—C4	178.9 (4)	Cu1—N1—C20—C19	−4.8 (4)
C2—C3—C4—C5	0.3 (6)	C11—C12—C20—N1	2.2 (6)
C3—C4—C5—C6	−0.2 (7)	C13—C12—C20—N1	−177.2 (4)
C3—C4—C5—C8	−179.4 (4)	C11—C12—C20—C19	−177.5 (4)
C4—C5—C6—C7	0.3 (6)	C13—C12—C20—C19	3.1 (6)

C8—C5—C6—C7	179.5 (4)	N2—C19—C20—N1	0.4 (5)
C5—C6—C7—C2	−0.4 (6)	C15—C19—C20—N1	179.4 (3)
C3—C2—C7—C6	0.5 (6)	N2—C19—C20—C12	−179.8 (3)
C1—C2—C7—C6	−178.9 (4)	C15—C19—C20—C12	−0.9 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2	0.85 (3)	1.696 (15)	2.520 (5)	164 (5)
O1W—H1W2···O6^{i}	0.85 (3)	1.870 (12)	2.714 (4)	175 (5)

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

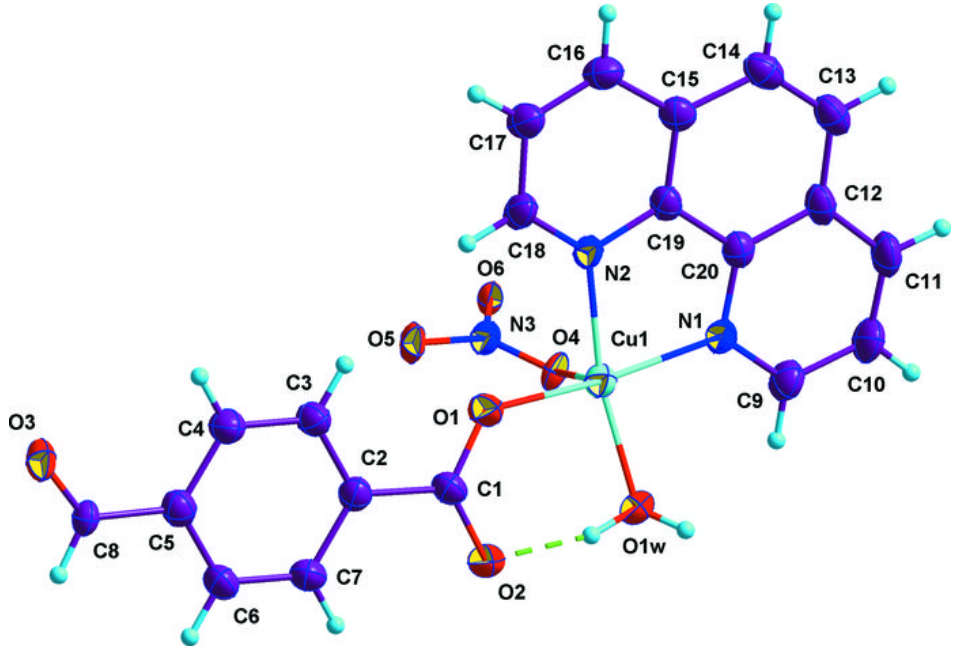
C16
C14
C15
C13
C17
C12
C18
C19
N2
C20
C11
O6
N3
O4
Cu1
N1
O5
C3
O1
C10
C9
O3
C4
C2
C1
C8
C5
O1w
C7
O2
C6

Fig. 2