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{2-[(2-Acetylhydrazin-1-ylidene)methyl-κ^2N^1,O]-6-methoxyphenolato-κO^1}-(nitrato-κO)copper(II) monohydrate

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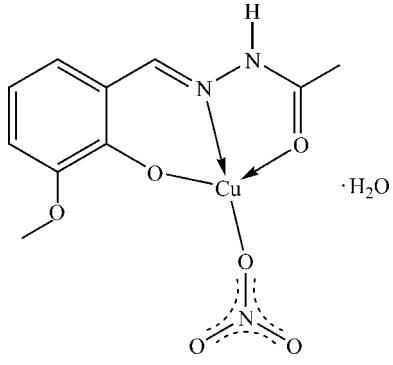
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 15.9.

In the title complex, $[Cu(C_{10}H_{11}N_2O_3)(NO_3)]\cdot H_2O$, prepared from the Schiff base N'-(3-methoxy-2-oxidobenzylidene)-acetohydrazide, the Cu^{II} atom is coordinated by two O atoms and one N atom from the ligand and one O atom from a nitrate group in a distorted square-planar geometry. The Cu^{II} atom has a weak interaction with another O atom of the nitrate group. The two O atoms of the tridentate Schiff base ligand are in a *trans* arrangement. O—H···O and N—H···O hydrogen bonds involving the uncoordinated water molecule are observed.

Related literature

For related structures, see: Ainscough *et al.* (1998); Koh *et al.* (1998); Tamboura *et al.* (2009); You & Zhu (2004).



Experimental

Crystal data

$[Cu(C_{10}H_{11}N_2O_3)(NO_3)]\cdot H_2O$
M_r = 350.77
Monoclinic, $P2_1/c$
a = 9.274 (2) Å
b = 10.455 (4) Å
c = 13.726 (4) Å
β = 95.16 (5)°
V = 1325.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 293 K
0.40 × 0.28 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.56, T_{max} = 0.72
5500 measured reflections
3046 independent reflections
2493 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.05
3046 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.9134 (18)	Cu1—O4	1.9663 (16)
Cu1—O1	1.8798 (15)	Cu1—O6	2.559 (2)
Cu1—O3	1.9730 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O7	0.86	1.95	2.801 (3)	174
O7—H1O···O1^{i}	0.92	2.40	3.271 (3)	159
O7—H1O···O2^{i}	0.92	2.42	3.050 (3)	126
O7—H2O···O5^{ii}	0.92	2.08	2.984 (3)	167

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2267).

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supporting information

Acta Cryst. (2010). E**66**, m136 [https://doi.org/10.1107/S1600536810000632]

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S1. Comment

In the title complex, the Cu^{II} ion adopts a four-coordinated geometry with the Schiff base coordinated to the metal ion as a uninegative charged tridentate ligand via the carbonyl O atom, the azomethine N atom and the phenolate O atom. The fourth coordination position is occupied by an O atom of the nitrate group. The Cu^{II} ion has a weak interaction with another O atom (O6) of the nitrate (Table 1). The bond distances of Cu—N and Cu—O are similar to the other Cu analogue with the same tridentate ligand (Ainscough *et al.*, 1998). The Cu—O(NO_3) distance is similar to the observed value for the complex [Cu(*L*)NO_3] [*L* = 1-(pyridin-2-ylmethyliminomethyl)naphtalen-2-olato] (You & Zhu, 2004). The two O donor atoms of the ligand are in a *trans* arrangement with an O—Cu—O angle of 173.76 (6)°. The angles around Cu are in a range of 81.49 (7)–173.76 (6)° and sum of the angles at Cu is 360.4°, suggesting that the geometry around the Cu atom is distorted square-planar (Fig. 1).

S2. Experimental

All purchased chemicals and solvents were reagent grade and used without further purification. The solid-state IR spectra were recorded from KBr discs on a Nicolet spectrophotometer. To a mixture of the ligand (0.211 g, 1.0 mmol) and 20 ml of ethanol was added dropwise a solution of copper nitrate dihydrate (0.242 g, 2.0 mmol) in 10 ml of ethanol. The resulting mixture was stirred under reflux for 2 h. After cooling the solution was filtered and the filtrate was left for slow evaporation. Green crystals of the title compound were obtained in good yield (0.290 g, 82.7%). IR (cm^{-1}): 3403, 1604, 1578, 1445, 1291, 1248, 1082, 1004, 331, 273. Melting point 196±1°C. Analysis, calculated for $C_{10}H_{13}CuN_3O_7$: C 34.24, H 3.74, N 11.98%; found: C 34.26, H 3.73, N 16.15%. Single crystals suitable for X-ray analysis were obtained from slow evaporation of a methanol solution of the product.

S3. Refinement

Water H atoms and amine H atoms of the Schiff base ligand were located from a difference Fourier map and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(N,O). Other H atoms were placed geometrically and refined with a riding model, with C—H = 0.93 (CH) and 0.96 (CH_3) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C).

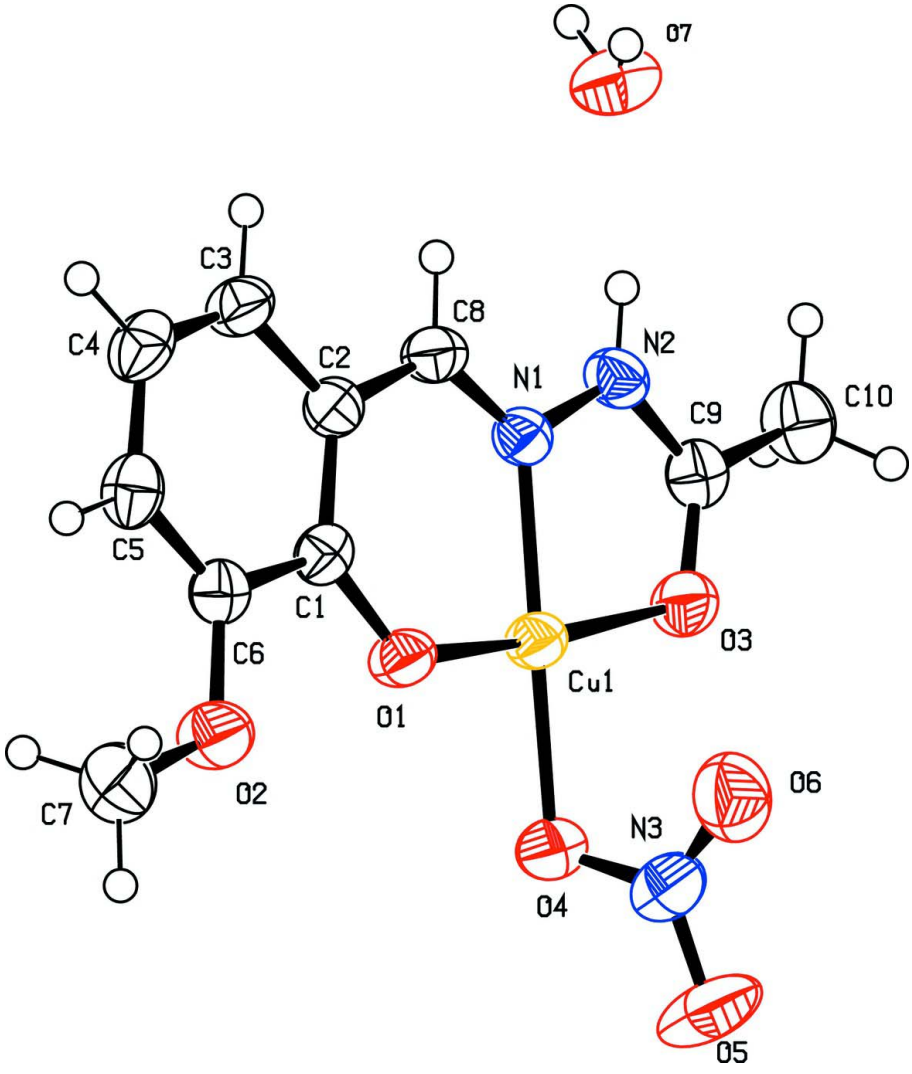

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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$b = 10.455$ (4) Å
$c = 13.726$ (4) Å
$\beta = 95.16$ (5)°
$V = 1325.5$ (7) Å^3
$Z = 4$

$F(000) = 716$
$D_x = 1.758$ Mg m^{-3}
Melting point: 469 K
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 12725 reflections
$\theta = 1.0$–27.5°
$\mu = 1.69$ mm^{-1}
$T = 293$ K
Prism, green
0.40 × 0.28 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.56, T_{max} = 0.72

5500 measured reflections
3046 independent reflections
2493 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −12→12
k = −13→12
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.05
3046 reflections
192 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
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.2512P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.09934 (3)	0.23847 (2)	0.104081 (19)	0.03448 (11)
O1	0.20916 (16)	0.08774 (13)	0.10007 (12)	0.0391 (3)
O2	0.39441 (16)	−0.09065 (15)	0.07532 (13)	0.0489 (4)
O3	−0.02563 (16)	0.38826 (14)	0.12039 (12)	0.0417 (4)
O4	0.25659 (17)	0.34556 (16)	0.06197 (12)	0.0464 (4)
O5	0.40681 (19)	0.48337 (19)	0.13003 (19)	0.0784 (7)
O6	0.2791 (2)	0.3648 (2)	0.21931 (14)	0.0662 (5)
O7	−0.45344 (19)	0.13264 (18)	0.18452 (13)	0.0589 (5)
H1O	−0.5371	0.1148	0.1455	0.071*
H2O	−0.4318	0.0772	0.2358	0.071*
N1	−0.07247 (18)	0.14998 (17)	0.13266 (12)	0.0321 (4)
N2	−0.1848 (2)	0.23436 (17)	0.14647 (14)	0.0362 (4)
H2N	−0.2694	0.2092	0.1591	0.043*
N3	0.31622 (19)	0.39954 (18)	0.13960 (18)	0.0477 (5)
C1	0.1588 (2)	−0.02931 (19)	0.10347 (14)	0.0323 (4)
C2	0.0145 (2)	−0.0638 (2)	0.11923 (14)	0.0336 (4)
C3	−0.0258 (3)	−0.1947 (2)	0.11989 (16)	0.0404 (5)
H3	−0.1210	−0.2163	0.1288	0.048*
C4	0.0720 (3)	−0.2894 (2)	0.10779 (16)	0.0435 (5)
H4	0.0438	−0.3747	0.1087	0.052*
C5	0.2160 (3)	−0.2570 (2)	0.09391 (17)	0.0405 (5)
H5	0.2833	−0.3214	0.0865	0.049*
C6	0.2581 (2)	−0.1313 (2)	0.09123 (15)	0.0351 (4)
C7	−0.0955 (2)	0.0287 (2)	0.13384 (15)	0.0360 (5)

H7	−0.1876	−0.0002	0.1447	0.043*
C8	0.5026 (3)	−0.1853 (3)	0.0650 (2)	0.0549 (6)
H8A	0.5203	−0.2318	0.1251	0.082*
H8B	0.5904	−0.1446	0.0494	0.082*
H8C	0.4699	−0.2432	0.0134	0.082*
C9	−0.1505 (2)	0.3575 (2)	0.13847 (15)	0.0371 (5)
C10	−0.2645 (3)	0.4550 (2)	0.14953 (19)	0.0504 (6)
H10A	−0.2274	0.5200	0.1944	0.076*
H10B	−0.3470	0.4149	0.1742	0.076*
H10C	−0.2929	0.4931	0.0871	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03077 (17)	0.02852 (15)	0.04481 (18)	−0.00120 (9)	0.00701 (11)	−0.00130 (10)
O1	0.0317 (8)	0.0291 (7)	0.0572 (9)	−0.0018 (6)	0.0082 (7)	−0.0017 (6)
O2	0.0358 (9)	0.0386 (9)	0.0730 (11)	0.0047 (7)	0.0088 (8)	−0.0013 (8)
O3	0.0378 (8)	0.0344 (8)	0.0534 (9)	0.0008 (6)	0.0068 (7)	−0.0025 (7)
O4	0.0435 (9)	0.0413 (9)	0.0556 (10)	−0.0083 (7)	0.0114 (7)	−0.0026 (7)
O5	0.0368 (10)	0.0432 (11)	0.154 (2)	−0.0105 (8)	0.0007 (12)	−0.0053 (12)
O6	0.0606 (12)	0.0783 (14)	0.0591 (12)	0.0034 (10)	0.0021 (10)	−0.0132 (10)
O7	0.0467 (10)	0.0621 (12)	0.0672 (12)	−0.0145 (8)	0.0010 (9)	0.0066 (9)
N1	0.0288 (8)	0.0329 (9)	0.0349 (9)	0.0014 (7)	0.0042 (7)	−0.0006 (7)
N2	0.0283 (9)	0.0406 (10)	0.0404 (10)	0.0032 (7)	0.0065 (8)	−0.0008 (7)
N3	0.0280 (9)	0.0326 (10)	0.0819 (16)	0.0059 (8)	0.0016 (10)	−0.0071 (10)
C1	0.0359 (11)	0.0303 (10)	0.0300 (10)	−0.0017 (8)	−0.0009 (8)	0.0011 (8)
C2	0.0366 (11)	0.0336 (10)	0.0304 (10)	−0.0023 (8)	0.0030 (8)	0.0009 (8)
C3	0.0422 (13)	0.0352 (12)	0.0439 (12)	−0.0087 (9)	0.0051 (10)	0.0011 (10)
C4	0.0575 (15)	0.0283 (10)	0.0442 (12)	−0.0059 (10)	0.0011 (11)	0.0021 (9)
C5	0.0499 (14)	0.0320 (11)	0.0386 (12)	0.0059 (9)	−0.0008 (10)	0.0000 (8)
C6	0.0358 (11)	0.0354 (11)	0.0335 (10)	0.0018 (9)	0.0011 (8)	−0.0005 (8)
C7	0.0315 (11)	0.0403 (12)	0.0364 (11)	−0.0064 (8)	0.0033 (9)	0.0012 (9)
C8	0.0411 (13)	0.0506 (15)	0.0730 (17)	0.0135 (11)	0.0048 (12)	−0.0068 (13)
C9	0.0374 (12)	0.0396 (11)	0.0337 (11)	0.0045 (9)	−0.0007 (8)	−0.0009 (9)
C10	0.0473 (14)	0.0481 (14)	0.0555 (14)	0.0140 (11)	0.0023 (11)	0.0005 (11)

Geometric parameters (Å, º)

Cu1—N1	1.9134 (18)	C1—C2	1.422 (3)
Cu1—O1	1.8798 (15)	C1—C6	1.428 (3)
Cu1—O3	1.9730 (16)	C2—C3	1.419 (3)
Cu1—O4	1.9663 (16)	C2—C7	1.433 (3)
Cu1—O6	2.559 (2)	C3—C4	1.363 (4)
O1—C1	1.312 (2)	C3—H3	0.9300
O2—C6	1.370 (3)	C4—C5	1.407 (3)
O2—C8	1.425 (3)	C4—H4	0.9300
O3—C9	1.248 (3)	C5—C6	1.373 (3)
O4—N3	1.286 (3)	C5—H5	0.9300

O5—N3	1.229 (3)	C7—H7	0.9300
O6—N3	1.231 (3)	C8—H8A	0.9600
O7—H1O	0.92	C8—H8B	0.9600
O7—H2O	0.92	C8—H8C	0.9600
N1—C7	1.286 (3)	C9—C10	1.486 (3)
N1—N2	1.391 (2)	C10—H10A	0.9600
N2—C9	1.333 (3)	C10—H10B	0.9600
N2—H2N	0.8600	C10—H10C	0.9600

O1—Cu1—N1	93.67 (7)	C4—C3—C2	121.4 (2)
O1—Cu1—O4	92.90 (7)	C4—C3—H3	119.3
N1—Cu1—O4	171.47 (7)	C2—C3—H3	119.3
O1—Cu1—O3	173.76 (6)	C3—C4—C5	119.5 (2)
N1—Cu1—O3	81.49 (7)	C3—C4—H4	120.3
O4—Cu1—O3	92.30 (7)	C5—C4—H4	120.3
O1—Cu1—O6	97.25 (7)	C6—C5—C4	120.7 (2)
O3—Cu1—O6	82.93 (7)	C6—C5—H5	119.7
O4—Cu1—O6	55.16 (7)	C4—C5—H5	119.7
N1—Cu1—O6	129.12 (7)	O2—C6—C5	124.8 (2)
C1—O1—Cu1	125.84 (13)	O2—C6—C1	113.64 (18)
C6—O2—C8	117.93 (18)	C5—C6—C1	121.6 (2)
C9—O3—Cu1	112.53 (14)	N1—C7—C2	122.85 (19)
N3—O4—Cu1	106.34 (13)	N1—C7—H7	118.6
H1O—O7—H2O	115.6	C2—C7—H7	118.6
C7—N1—N2	119.75 (18)	O2—C8—H8A	109.5
C7—N1—Cu1	128.43 (15)	O2—C8—H8B	109.5
N2—N1—Cu1	111.66 (13)	H8A—C8—H8B	109.5
C9—N2—N1	114.45 (17)	O2—C8—H8C	109.5
C9—N2—H2N	122.8	H8A—C8—H8C	109.5
N1—N2—H2N	122.8	H8B—C8—H8C	109.5
O5—N3—O6	123.6 (2)	O3—C9—N2	119.85 (19)
O5—N3—O4	118.1 (2)	O3—C9—C10	121.7 (2)
O6—N3—O4	118.24 (19)	N2—C9—C10	118.4 (2)
O1—C1—C2	125.80 (19)	C9—C10—H10A	109.5
O1—C1—C6	117.19 (18)	C9—C10—H10B	109.5
C2—C1—C6	117.01 (18)	H10A—C10—H10B	109.5
C3—C2—C1	119.86 (19)	C9—C10—H10C	109.5
C3—C2—C7	117.3 (2)	H10A—C10—H10C	109.5
C1—C2—C7	122.82 (19)	H10B—C10—H10C	109.5

N1—Cu1—O1—C1	7.99 (17)	C1—C2—C3—C4	1.5 (3)
O4—Cu1—O1—C1	−166.57 (17)	C7—C2—C3—C4	−179.2 (2)
N1—Cu1—O3—C9	−1.29 (15)	C2—C3—C4—C5	−0.3 (3)
O4—Cu1—O3—C9	172.83 (15)	C3—C4—C5—C6	−0.8 (4)
O1—Cu1—O4—N3	−101.08 (13)	C8—O2—C6—C5	−2.9 (3)
O3—Cu1—O4—N3	75.48 (14)	C8—O2—C6—C1	178.26 (19)
O1—Cu1—N1—C7	−7.63 (19)	C4—C5—C6—O2	−178.0 (2)
O3—Cu1—N1—C7	176.33 (18)	C4—C5—C6—C1	0.7 (3)

O1—Cu1—N1—N2	177.15 (13)	O1—C1—C6—O2	−1.3 (3)
O3—Cu1—N1—N2	1.11 (13)	C2—C1—C6—O2	179.32 (18)
C7—N1—N2—C9	−176.51 (19)	O1—C1—C6—C5	179.8 (2)
Cu1—N1—N2—C9	−0.8 (2)	C2—C1—C6—C5	0.4 (3)
Cu1—O4—N3—O5	−171.45 (16)	N2—N1—C7—C2	179.38 (18)
Cu1—O4—N3—O6	8.3 (2)	Cu1—N1—C7—C2	4.5 (3)
Cu1—O1—C1—C2	−5.8 (3)	C3—C2—C7—N1	−178.50 (19)
Cu1—O1—C1—C6	174.91 (14)	C1—C2—C7—N1	0.8 (3)
O1—C1—C2—C3	179.18 (19)	Cu1—O3—C9—N2	1.2 (3)
C6—C1—C2—C3	−1.5 (3)	Cu1—O3—C9—C10	−177.50 (16)
O1—C1—C2—C7	−0.1 (3)	N1—N2—C9—O3	−0.3 (3)
C6—C1—C2—C7	179.19 (18)	N1—N2—C9—C10	178.48 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O7	0.86	1.95	2.801 (3)	174
O7—H1*O*···O1^{i}	0.92	2.40	3.271 (3)	159
O7—H1*O*···O2^{i}	0.92	2.42	3.050 (3)	126
O7—H2*O*···O5^{ii}	0.92	2.08	2.984 (3)	167

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