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[1,2-Bis(2-pyridylmethoxy)benzene-κ^4N,O,O',N']bis(nitrato-κO)copper(II)

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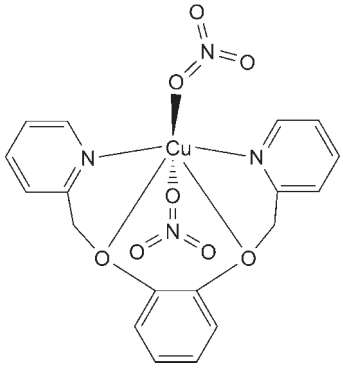
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.111; data-to-parameter ratio = 15.4.

In the title compound, $[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)]$, the Cu^{II} ion is six-coordinated in a Jahn–Teller-distorted octahedral environment defined by two O and two N atoms from the ligand and two O atoms from two monodentate nitrate anions.

Related literature

For the synthesis and general backround to flexible pyridyl-based ligands, see: Liu *et al.* (2010). For a related structure, see: Zhang *et al.* (2010).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)]$
M_r = 479.90
Triclinic, $P\overline{1}$
a = 8.621 (5) Å
b = 10.826 (6) Å
c = 10.887 (6) Å
α = 78.75 (2)°
β = 77.590 (19)°
γ = 76.54 (2)°
V = 953.8 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 291 K
0.31 × 0.30 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.705, T_{max} = 0.808
9416 measured reflections
4314 independent reflections
3150 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.111
S = 1.04
4314 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O3	1.968 (2)	Cu1—N2	2.070 (2)
Cu1—O6	1.973 (2)	Cu1—O2	2.451 (3)
Cu1—N1	2.062 (3)	Cu1—O1	2.491 (2)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2792).

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supporting information

Acta Cryst. (2010). E**66**, m872 [https://doi.org/10.1107/S1600536810024773]

[1,2-Bis(2-pyridylmethoxy)benzene-κ^4N,O,O',N']bis(nitrato-κO)copper(II)

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S1. Comment

In recent, our group has employed the flexible N-heterocyclic ligands reacting with transition metal to construct several supramolecular architectures (Liu *et al.* 2010; Zhang *et al.* 2010). As a part of our continuing work for bipyridyl aromatic ligands, we report the crystal s tructure of the title compound here.

1,2-Bis(pyridin-2-ylmethoxy)benzene molecule act as a chelating ligand to coordinate with Cu^{II} ion forming a discrete strucutre. Two nitrate anions also coordinate to the center Cu^{II} ion, resulting the Cu^{II} ion is six-coordinated in a typically Jahn-Teller distorted octahedral environment. Furthermore, a weak Cu—O bond, with distances of 2.742 (3) Å, between the Cu^{II} center and one nitrate anion link the coordination geometry into a distorted monocapped octahedron (Figure 1, Table 1).

S2. Experimental

The 1,2-Bis(pyridin-2-ylmethoxy)benzene was synthesized by the reaction of *o*-dihydroxybenzene and 2-chloromethyl-pyridine hydrochloride under nitrogen atmosphere and alkaline condition (Liu *et al.*, 2010). Title ligand (0.58 g, 2 mmol) and $Cu(NO_3)_2{\cdot}H_2O$ (0.48 g, 2 mmol) were dissolved in 15 ml e thanol, and then the mixture keep stirring for 30 minute. The resulting solution was filtered, and the filtrate was allowed to stand in a desiccator at room temperature for several days. Bule block crystals were obtained.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methene C), and with U_{iso}(H) = *1.2*U_{eq}(C).

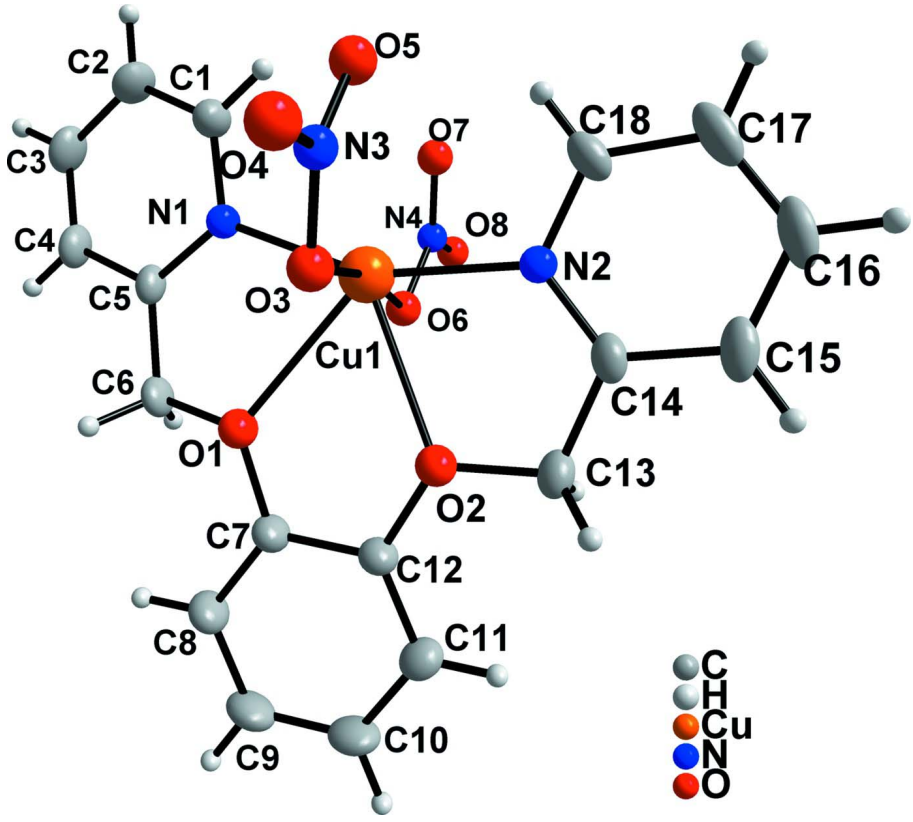

Figure 1

The molecular structure of title compound, showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

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Crystal data

$[Cu(NO_3)_2(C_{18}H_{16}N_2O_2)]$
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$c = 10.887$ (6) Å
$\alpha = 78.75$ (2)°
$\beta = 77.590$ (19)°
$\gamma = 76.54$ (2)°
$V = 953.8$ (9) Å^3
$Z = 2$
$F(000) = 490$
$D_x = 1.671$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6858 reflections
$\theta = 3.4$–27.5°
$\mu = 1.20$ mm^{-1}
$T = 291$ K
Block, blue
0.31 × 0.30 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.705$, $T_{max} = 0.808$
9416 measured reflections
4314 independent reflections
3150 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -11 \rightarrow 10$
$k = -13 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.111$
$S = 1.04$
4314 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.2381P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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}
C1	0.5717 (4)	0.6307 (3)	0.2015 (3)	0.0476 (8)
H1	0.5016	0.5749	0.2394	0.057*
C2	0.7258 (4)	0.5802 (4)	0.1445 (3)	0.0562 (9)
H2	0.7589	0.4923	0.1434	0.067*
C3	0.8307 (4)	0.6624 (4)	0.0890 (3)	0.0551 (9)
H3	0.9350	0.6308	0.0486	0.066*
C4	0.7797 (4)	0.7903 (4)	0.0941 (3)	0.0483 (8)
H4	0.8498	0.8465	0.0582	0.058*
C5	0.6229 (3)	0.8369 (3)	0.1529 (3)	0.0379 (7)
C6	0.5702 (3)	0.9769 (3)	0.1585 (3)	0.0437 (7)
H6A	0.6479	1.0057	0.1933	0.052*
H6B	0.5667	1.0237	0.0732	0.052*
C7	0.3364 (4)	1.1288 (3)	0.2277 (3)	0.0438 (7)
C8	0.4092 (4)	1.2346 (3)	0.1885 (3)	0.0523 (8)
H8	0.5211	1.2240	0.1634	0.063*
C9	0.3133 (5)	1.3562 (4)	0.1871 (4)	0.0620 (10)
H9	0.3610	1.4279	0.1607	0.074*
C10	0.1485 (5)	1.3722 (4)	0.2244 (3)	0.0586 (9)
H10	0.0852	1.4546	0.2224	0.070*
C11	0.0755 (4)	1.2666 (3)	0.2649 (3)	0.0490 (8)
H11	−0.0363	1.2776	0.2898	0.059*
C12	0.1699 (4)	1.1457 (3)	0.2678 (3)	0.0424 (7)
C13	−0.0517 (4)	1.0379 (3)	0.3337 (3)	0.0481 (8)
H13A	−0.0955	1.0785	0.2574	0.058*
H13B	−0.1040	1.0888	0.4009	0.058*

C14	−0.0837 (3)	0.9041 (3)	0.3722 (3)	0.0407 (7)
C15	−0.2393 (4)	0.8881 (4)	0.4305 (3)	0.0555 (10)
H15	−0.3201	0.9587	0.4495	0.067*
C16	−0.2722 (4)	0.7667 (5)	0.4595 (3)	0.0633 (11)
H16	−0.3756	0.7541	0.4984	0.076*
C17	−0.1513 (5)	0.6645 (4)	0.4307 (3)	0.0626 (11)
H17	−0.1724	0.5819	0.4475	0.075*
C18	0.0027 (4)	0.6850 (4)	0.3761 (3)	0.0486 (8)
H18	0.0850	0.6147	0.3588	0.058*
Cu1	0.27619 (4)	0.81850 (4)	0.27623 (3)	0.03697 (13)
N1	0.5180 (3)	0.7571 (3)	0.2049 (2)	0.0391 (6)
N2	0.0374 (3)	0.8036 (3)	0.3473 (2)	0.0399 (6)
N3	0.3327 (3)	0.6879 (3)	0.5135 (3)	0.0522 (7)
N4	0.2099 (3)	0.7793 (3)	0.0525 (3)	0.0485 (7)
O1	0.4174 (3)	1.0028 (2)	0.2342 (2)	0.0579 (7)
O2	0.1161 (3)	1.0317 (2)	0.3109 (2)	0.0541 (6)
O3	0.3212 (3)	0.8020 (2)	0.4491 (2)	0.0479 (5)
O4	0.3539 (4)	0.6751 (3)	0.6242 (2)	0.0797 (9)
O5	0.3246 (3)	0.5986 (3)	0.4623 (3)	0.0697 (7)
O6	0.2278 (3)	0.8736 (2)	0.1024 (2)	0.0483 (5)
O7	0.2304 (3)	0.6710 (3)	0.1141 (2)	0.0646 (7)
O8	0.1728 (3)	0.8034 (3)	−0.0531 (2)	0.0794 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0415 (17)	0.044 (2)	0.0546 (19)	−0.0102 (15)	−0.0042 (15)	−0.0046 (15)
C2	0.049 (2)	0.052 (2)	0.062 (2)	0.0012 (16)	−0.0054 (17)	−0.0134 (17)
C3	0.0343 (17)	0.074 (3)	0.0494 (19)	−0.0028 (17)	0.0021 (15)	−0.0115 (18)
C4	0.0292 (15)	0.064 (2)	0.0468 (17)	−0.0116 (15)	−0.0014 (14)	0.0001 (16)
C5	0.0279 (14)	0.0487 (19)	0.0345 (14)	−0.0105 (13)	−0.0050 (12)	0.0028 (13)
C6	0.0327 (15)	0.050 (2)	0.0473 (17)	−0.0182 (14)	−0.0010 (14)	−0.0005 (14)
C7	0.0417 (16)	0.0371 (18)	0.0511 (18)	−0.0123 (14)	−0.0040 (14)	−0.0024 (14)
C8	0.0495 (19)	0.047 (2)	0.060 (2)	−0.0182 (16)	−0.0063 (16)	−0.0008 (16)
C9	0.078 (3)	0.040 (2)	0.075 (2)	−0.0217 (19)	−0.018 (2)	−0.0074 (18)
C10	0.078 (3)	0.0350 (19)	0.064 (2)	−0.0062 (18)	−0.020 (2)	−0.0064 (16)
C11	0.0487 (19)	0.047 (2)	0.0480 (18)	−0.0010 (15)	−0.0106 (15)	−0.0081 (15)
C12	0.0436 (17)	0.0357 (17)	0.0473 (17)	−0.0096 (14)	−0.0070 (14)	−0.0036 (13)
C13	0.0330 (16)	0.056 (2)	0.0500 (18)	−0.0058 (14)	−0.0041 (14)	−0.0025 (16)
C14	0.0326 (15)	0.059 (2)	0.0325 (14)	−0.0162 (15)	−0.0063 (12)	−0.0020 (14)
C15	0.0326 (16)	0.091 (3)	0.0423 (17)	−0.0185 (18)	−0.0011 (14)	−0.0079 (18)
C16	0.0415 (19)	0.107 (3)	0.049 (2)	−0.042 (2)	−0.0039 (16)	0.001 (2)
C17	0.066 (2)	0.088 (3)	0.0475 (19)	−0.054 (2)	−0.0157 (18)	0.0114 (19)
C18	0.0539 (19)	0.056 (2)	0.0432 (17)	−0.0319 (17)	−0.0090 (15)	0.0012 (15)
Cu1	0.02889 (19)	0.0399 (2)	0.0400 (2)	−0.01305 (15)	0.00069 (14)	−0.00118 (15)
N1	0.0303 (12)	0.0465 (16)	0.0378 (13)	−0.0102 (11)	−0.0027 (10)	−0.0007 (11)
N2	0.0350 (13)	0.0520 (16)	0.0342 (12)	−0.0213 (12)	−0.0021 (11)	0.0005 (11)
N3	0.0310 (13)	0.065 (2)	0.0543 (17)	−0.0149 (13)	0.0011 (13)	0.0023 (15)

N4	0.0308 (13)	0.071 (2)	0.0424 (15)	−0.0182 (14)	−0.0001 (12)	−0.0039 (15)
O1	0.0366 (12)	0.0384 (13)	0.0859 (17)	−0.0129 (10)	0.0161 (12)	−0.0025 (12)
O2	0.0341 (11)	0.0381 (13)	0.0834 (17)	−0.0103 (10)	0.0038 (11)	−0.0055 (12)
O3	0.0424 (12)	0.0532 (15)	0.0473 (12)	−0.0145 (11)	−0.0035 (10)	−0.0044 (11)
O4	0.0758 (19)	0.110 (3)	0.0458 (15)	−0.0190 (18)	−0.0146 (14)	0.0102 (15)
O5	0.0650 (17)	0.0577 (18)	0.0864 (19)	−0.0236 (14)	−0.0116 (15)	0.0006 (15)
O6	0.0458 (12)	0.0476 (14)	0.0471 (12)	−0.0159 (11)	−0.0040 (10)	0.0069 (10)
O7	0.0703 (17)	0.0573 (17)	0.0655 (16)	−0.0189 (14)	−0.0083 (13)	−0.0044 (14)
O8	0.0679 (18)	0.134 (3)	0.0429 (14)	−0.0424 (19)	−0.0161 (13)	0.0037 (15)

Geometric parameters (Å, º)

C1—N1	1.344 (4)	C13—C14	1.500 (5)
C1—C2	1.374 (4)	C13—H13A	0.9700
C1—H1	0.9300	C13—H13B	0.9700
C2—C3	1.380 (5)	C14—N2	1.346 (4)
C2—H2	0.9300	C14—C15	1.390 (4)
C3—C4	1.359 (5)	C15—C16	1.371 (6)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.389 (4)	C16—C17	1.366 (6)
C4—H4	0.9300	C16—H16	0.9300
C5—N1	1.355 (4)	C17—C18	1.383 (4)
C5—C6	1.487 (5)	C17—H17	0.9300
C6—O1	1.395 (3)	C18—N2	1.348 (4)
C6—H6A	0.9700	C18—H18	0.9300
C6—H6B	0.9700	Cu1—O3	1.968 (2)
C7—O1	1.376 (4)	Cu1—O6	1.973 (2)
C7—C8	1.385 (4)	Cu1—N1	2.062 (3)
C7—C12	1.387 (4)	Cu1—N2	2.070 (2)
C8—C9	1.381 (5)	Cu1—O2	2.451 (3)
C8—H8	0.9300	Cu1—O1	2.491 (2)
C9—C10	1.371 (5)	Cu1—O7	2.742 (3)
C9—H9	0.9300	N3—O5	1.229 (4)
C10—C11	1.384 (5)	N3—O4	1.233 (4)
C10—H10	0.9300	N3—O3	1.290 (4)
C11—C12	1.370 (5)	N4—O8	1.223 (4)
C11—H11	0.9300	N4—O7	1.226 (4)
C12—O2	1.380 (4)	N4—O6	1.298 (4)
C13—O2	1.403 (4)		

N1—C1—C2	122.8 (3)	C17—C16—C15	119.2 (3)
N1—C1—H1	118.6	C17—C16—H16	120.4
C2—C1—H1	118.6	C15—C16—H16	120.4
C1—C2—C3	118.8 (3)	C16—C17—C18	119.5 (4)
C1—C2—H2	120.6	C16—C17—H17	120.3
C3—C2—H2	120.6	C18—C17—H17	120.3
C4—C3—C2	119.2 (3)	N2—C18—C17	122.1 (4)
C4—C3—H3	120.4	N2—C18—H18	119.0

C2—C3—H3	120.4	C17—C18—H18	119.0
C3—C4—C5	120.0 (3)	O3—Cu1—O6	168.05 (10)
C3—C4—H4	120.0	O3—Cu1—N1	91.68 (10)
C5—C4—H4	120.0	O6—Cu1—N1	90.92 (10)
N1—C5—C4	121.1 (3)	O3—Cu1—N2	91.37 (9)
N1—C5—C6	119.8 (3)	O6—Cu1—N2	90.77 (10)
C4—C5—C6	119.1 (3)	N1—Cu1—N2	157.09 (11)
O1—C6—C5	110.5 (2)	O3—Cu1—O2	85.99 (10)
O1—C6—H6A	109.5	O6—Cu1—O2	83.59 (10)
C5—C6—H6A	109.5	N1—Cu1—O2	131.82 (9)
O1—C6—H6B	109.5	N2—Cu1—O2	71.06 (9)
C5—C6—H6B	109.5	O3—Cu1—O1	83.11 (9)
H6A—C6—H6B	108.1	O6—Cu1—O1	86.74 (9)
O1—C7—C8	125.0 (3)	N1—Cu1—O1	70.71 (9)
O1—C7—C12	114.9 (3)	N2—Cu1—O1	132.20 (9)
C8—C7—C12	120.0 (3)	O2—Cu1—O1	61.22 (8)
C9—C8—C7	119.0 (3)	O3—Cu1—O7	140.28 (9)
C9—C8—H8	120.5	O6—Cu1—O7	51.65 (10)
C7—C8—H8	120.5	N1—Cu1—O7	83.49 (10)
C10—C9—C8	120.6 (3)	N2—Cu1—O7	79.70 (9)
C10—C9—H9	119.7	O2—Cu1—O7	125.77 (9)
C8—C9—H9	119.7	O1—Cu1—O7	130.79 (8)
C9—C10—C11	120.5 (4)	C1—N1—C5	118.1 (3)
C9—C10—H10	119.8	C1—N1—Cu1	117.6 (2)
C11—C10—H10	119.8	C5—N1—Cu1	124.1 (2)
C12—C11—C10	119.3 (3)	C14—N2—C18	118.0 (3)
C12—C11—H11	120.4	C14—N2—Cu1	124.1 (2)
C10—C11—H11	120.4	C18—N2—Cu1	117.8 (2)
C11—C12—O2	126.0 (3)	O5—N3—O4	123.7 (3)
C11—C12—C7	120.5 (3)	O5—N3—O3	119.2 (3)
O2—C12—C7	113.4 (3)	O4—N3—O3	117.0 (3)
O2—C13—C14	108.8 (3)	O8—N4—O7	123.4 (3)
O2—C13—H13A	109.9	O8—N4—O6	118.3 (3)
C14—C13—H13A	109.9	O7—N4—O6	118.3 (3)
O2—C13—H13B	109.9	C7—O1—C6	117.7 (2)
C14—C13—H13B	109.9	C7—O1—Cu1	123.01 (18)
H13A—C13—H13B	108.3	C6—O1—Cu1	112.23 (19)
N2—C14—C15	122.0 (3)	C12—O2—C13	117.3 (3)
N2—C14—C13	119.4 (2)	C12—O2—Cu1	124.99 (18)
C15—C14—C13	118.6 (3)	C13—O2—Cu1	113.57 (19)
C16—C15—C14	119.1 (4)	N3—O3—Cu1	115.3 (2)
C16—C15—H15	120.4	N4—O6—Cu1	112.66 (19)
C14—C15—H15	120.4	N4—O7—Cu1	77.37 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*B*···O6^{i}	0.97	2.58	3.333 (4)	135

C13—H13*A*···O8^{ii}	0.97	2.48	3.444 (5)	172
C13—H13*B*···O3^{iii}	0.97	2.45	3.370 (4)	159
C17—H17···O5^{iv}	0.93	2.53	3.412 (5)	159

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