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Aquabis(3,5-dimethyl-1*H*-pyrazole-κ*N*)-(oxalato-κ^2*O*,*O*′)copper(II)

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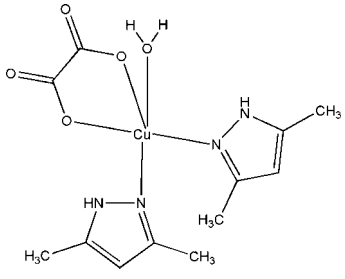
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.070; wR factor = 0.175; data-to-parameter ratio = 18.5.

In the title compound, $[Cu(C_2O_4)(C_5H_8N_2)_2(H_2O)]$, the Cu^{II} atom is coordinated in a slightly distorted square-pyramidal geometry by two N atoms belonging to the two 3,5-dimethyl-1*H*-pyrazole ligands, two O atoms of the oxalate anion providing an *O*,*O*′-chelating coordination mode, and an O atom of the water molecule occupying the apical position. The crystal packing shows a well defined layer structure. Intra-layer connections are realised through a system of hydrogen bonds while the nature of the inter-layer interactions is completely hydrophobic, including no hydrogen-bonding interactions.

Related literature

For related literature on metal oxalates and 1*H*-pyrazole complexes, see: Abdeljalil *et al.* (2006); Bataille & Louër (1999); Castillo *et al.* (2001); Naumov *et al.* (1995); Raptis *et al.* (1999); Strotmeyer *et al.* (2003); Tomyn *et al.* (2007); Warda (1998).



Experimental

Crystal data

$[Cu(C_2O_4)(C_5H_8N_2)_2(H_2O)]$
M_r = 361.84
Triclinic, $P\overline{1}$
a = 8.2597 (6) Å
b = 8.4010 (8) Å
c = 12.2288 (11) Å
α = 77.007 (4)°
β = 89.189 (6)°
γ = 62.436 (5)°
V = 729.00 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 120 (2) K
0.23 × 0.13 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.720, T_{max} = 0.888
11529 measured reflections
3765 independent reflections
3186 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.175
S = 1.12
3765 reflections
204 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.946 (2)	Cu1—N3	2.002 (2)
Cu1—O5	1.971 (2)	Cu1—O1	2.283 (2)
Cu1—N2	1.975 (3)		
O2—Cu1—O5	84.54 (9)	N2—Cu1—N3	93.53 (10)
O2—Cu1—N2	172.35 (10)	O2—Cu1—O1	89.05 (9)
O5—Cu1—N2	92.59 (9)	O5—Cu1—O1	91.85 (9)
O2—Cu1—N3	88.41 (10)	N2—Cu1—O1	98.15 (10)
O5—Cu1—N3	170.11 (10)	N3—Cu1—O1	94.96 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.99	1.88	2.798 (3)	153
O1—H2···O5^{ii}	0.97	1.97	2.923 (3)	168
N1—H3···O3^{iii}	0.88	2.03	2.857 (3)	156
N4—H18···O3^{i}	0.88	1.97	2.845 (3)	175

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2100).

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supporting information

Acta Cryst. (2008). E**64**, m37–m38 [https://doi.org/10.1107/S1600536807058928]

Aquabis(3,5-dimethyl-1*H*-pyrazole-κN)(oxalato-$\kappa^2 O,O'$)copper(II)

Andrii I. Buvailo, Stefania V. Tomyn, Matti Haukka, Vadim A. Pavlenko and Igor O. Fritsky

S1. Comment

1*H*-Pyrazole and its 3,5-substituted derivatives have been widely used as bridging ligands in molecular magnetism and supramolecular chemistry for obtaining discrete oligonuclear complexes of high nuclearity and coordination polymers (Abdeljalil *et al.*, 2006; Raptis *et al.*, 1999; Warda, 1998). On the other hand, oxalate is an important polynucleative ligand as it can exhibit various bridging modes, which, together with the varied coordination preferences of metal ions, can result in the formation of oligonuclear species or compounds containing one-, two- and three-dimensional coordination polymers and frameworks (Castillo *et al.*, 2001; Naumov *et al.*, 1995; Bataille & Louër, 1999; Strotmeyer *et al.*, 2003; Tomyn *et al.*, 2007). Simultanetous use of 1*H*-pyrazole derivatives and oxalates can result in the creation of new molecular topologies or in obtaining mononuclear complexes with vacant donor atoms, which can be used as building blocks for the preparation of oligonuclear assemblies or coordination polymers.

The molecular structure of the title compound (Fig. 1) consists of a Cu^{II} ion as the central atom possessing a slightly distorted square-pyramidal geometry. The four equatorial positions are occupied by two N atoms belonging to the two monodentately coordinated 3,5-dimethyl-1*H*-pyrazole molecules and two O atoms of the oxalate anion coordinated in an O,*O*′-chelate mode forming a five-membered chelate ring. The axial position is occupied by the O atom of the water molecule (Table 1). A crystal packing diagram (Fig. 2) depicts a well defined layer structure along the *c*-axis direction. Each layer is formed with the help of O1—H···O and N—H···O hydrogen bonds (Table 2) while the nature of inter-layer interactions is utterly hydrophobic including no hydrogen bonding interactions.

S2. Experimental

$Cu(NO_3)_2.3H_2O$ (0.242 g, 1 mmol) and 3,5-dimethyl-1*H*-pyrazole (0.961 g, 1 mmol) were dissolved in water (10 ml), and then a powder of $K_2C_2O_4.H_2O$ (0.184 g, 1 mmol) was added to the obtained solution. The resulting mixture was stirred at 358 K for 25 min and filtered. Blue needle-like crystals suitable for X-ray analysis were formed from the filtrate in several minutes. They were filtered off and washed with diethyl ester (yield 67%). Analysis calculated for $C_{12}H_{18}CuN_4O_5$: C 39.83, H 5.01, N 15.48%; found: C 39.11, H 5.13, N 15.42%.

S3. Refinement

H atoms on the ligand were positioned geometrically and refined as riding atoms, with C—H = 0.95Å (CH), 0.98Å (CH_3), N—H = 0.88Å and with U_{iso}(H) = 1.5U_{eq}(C) for methyl groups and U_{iso}(H) = 1.2U_{eq}(C, N) for the others. H atoms of the water molecule were located from a difference Fourier map and fixed with U_{iso}(H) = 1.5U_{eq}(O). The structure was refined as twinned. BASF parameter was refined to 0.307.

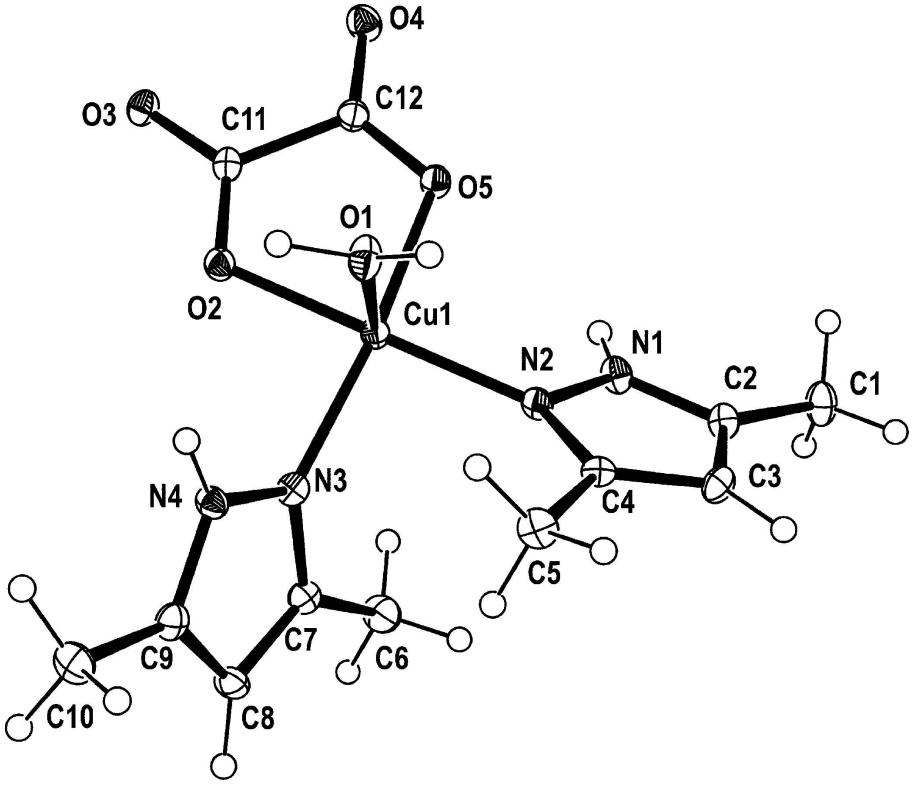

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are shown at the 30% probability level.

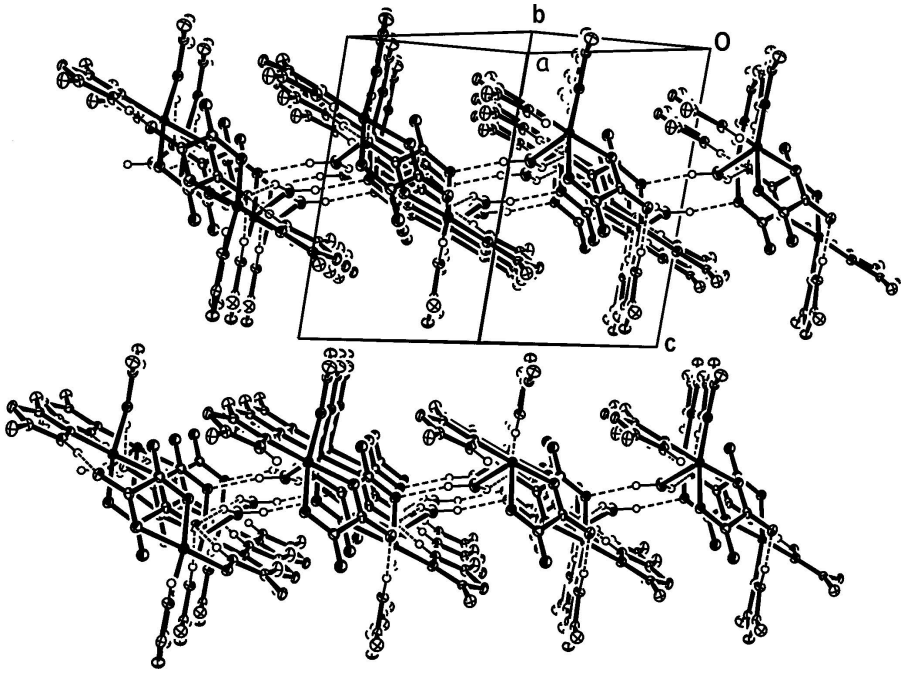

Figure 2

A packing diagram for the title compound, showing the layers along the *c*-axis direction. Hydrogen bonds are indicated by dashed lines. H atoms not included in hydrogen bonds are omitted for clarity.

Aquabis(3,5-dimethyl-1*H*-pyrazole-κN)(oxalato-κ^2O,O')copper(II)

Crystal data

$[Cu(C_2O_4)(C_5H_8N_2)_2(H_2O)]$
$M_r = 361.84$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2597$ (6) Å
$b = 8.4010$ (8) Å
$c = 12.2288$ (11) Å
$\alpha = 77.007$ (4)°
$\beta = 89.189$ (6)°
$\gamma = 62.436$ (5)°
$V = 729.00$ (11) Å^3
$Z = 2$
$F(000) = 374$
$D_x = 1.648$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 33067 reflections
$\theta = 1.0$–$27.5°$
$\mu = 1.53$ mm^{-1}
$T = 120$ K
Plate, blue
0.23 × 0.13 × 0.08 mm

Data collection

Nonius Kappa CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.720$, $T_{max} = 0.888$
11529 measured reflections
3765 independent reflections
3186 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 28.7°$, $\theta_{min} = 2.8°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.175$
$S = 1.12$
3765 reflections
204 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
$w = 1/[\sigma^2(F_o^2) + 4.1563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -1.02$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.14007 (5)	0.12441 (5)	0.63070 (3)	0.01550 (12)
O5	−0.0055 (3)	0.3021 (3)	0.48971 (18)	0.0169 (5)
O2	0.3431 (3)	0.1554 (3)	0.56547 (17)	0.0177 (5)
O4	0.0332 (3)	0.4796 (3)	0.33510 (18)	0.0224 (5)
O3	0.3977 (3)	0.3252 (3)	0.41587 (18)	0.0185 (5)
O1	0.2189 (3)	−0.1213 (3)	0.55296 (19)	0.0228 (5)
H1	0.3490	−0.1861	0.5383	0.034*
H2	0.1570	−0.1934	0.5482	0.034*
N2	−0.0797 (3)	0.1276 (3)	0.6984 (2)	0.0158 (5)
N1	−0.2437 (3)	0.2848 (4)	0.6778 (2)	0.0180 (6)
H3	−0.2596	0.3944	0.6406	0.022*
N3	0.3058 (3)	−0.0261 (4)	0.7738 (2)	0.0160 (5)

N4	0.4574 (3)	−0.1886 (3)	0.7756 (2)	0.0163 (5)
H18	0.4959	−0.2313	0.7156	0.020*
C2	−0.3788 (4)	0.2518 (4)	0.7215 (3)	0.0171 (6)
C1	−0.5724 (4)	0.4006 (5)	0.7112 (3)	0.0237 (7)
H4	−0.5811	0.4835	0.7587	0.036*
H6	−0.6521	0.3449	0.7358	0.036*
H5	−0.6112	0.4715	0.6324	0.036*
C3	−0.2992 (4)	0.0638 (4)	0.7711 (3)	0.0185 (7)
H7	−0.3591	−0.0028	0.8086	0.022*
C4	−0.1140 (4)	−0.0081 (4)	0.7551 (2)	0.0146 (6)
C5	0.0343 (4)	−0.2053 (4)	0.7949 (3)	0.0202 (7)
H10	0.1196	−0.2364	0.7372	0.030*
H8	−0.0210	−0.2881	0.8083	0.030*
H9	0.1011	−0.2201	0.8652	0.030*
C9	0.5419 (4)	−0.2766 (4)	0.8815 (3)	0.0183 (7)
C10	0.7136 (4)	−0.4587 (4)	0.9037 (3)	0.0229 (7)
H15	0.6822	−0.5597	0.9263	0.034*
H16	0.7949	−0.4659	0.9642	0.034*
H17	0.7761	−0.4698	0.8349	0.034*
C8	0.4410 (4)	−0.1676 (4)	0.9506 (3)	0.0189 (7)
H14	0.4654	−0.1924	1.0300	0.023*
C7	0.2938 (4)	−0.0112 (4)	0.8806 (3)	0.0172 (6)
C6	0.1419 (4)	0.1515 (5)	0.9110 (3)	0.0243 (7)
H12	0.0974	0.2589	0.8460	0.036*
H13	0.1869	0.1792	0.9743	0.036*
H11	0.0414	0.1238	0.9329	0.036*
C11	0.2947 (4)	0.2729 (4)	0.4716 (2)	0.0149 (6)
C12	0.0885 (4)	0.3626 (4)	0.4252 (3)	0.0176 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01345 (19)	0.0151 (2)	0.0170 (2)	−0.00671 (15)	0.00082 (14)	−0.00214 (15)
O5	0.0149 (10)	0.0147 (11)	0.0191 (11)	−0.0066 (9)	0.0009 (8)	−0.0013 (9)
O2	0.0150 (11)	0.0167 (12)	0.0189 (11)	−0.0065 (9)	0.0008 (9)	−0.0018 (9)
O4	0.0206 (11)	0.0199 (12)	0.0237 (12)	−0.0091 (10)	−0.0018 (9)	−0.0005 (10)
O3	0.0181 (11)	0.0157 (12)	0.0221 (11)	−0.0089 (9)	0.0044 (9)	−0.0036 (9)
O1	0.0174 (11)	0.0246 (13)	0.0310 (13)	−0.0107 (10)	0.0065 (9)	−0.0138 (10)
N2	0.0137 (12)	0.0110 (13)	0.0179 (13)	−0.0032 (10)	−0.0006 (10)	−0.0005 (10)
N1	0.0147 (13)	0.0114 (13)	0.0245 (14)	−0.0039 (11)	−0.0004 (11)	−0.0033 (11)
N3	0.0174 (13)	0.0135 (13)	0.0179 (13)	−0.0075 (11)	0.0032 (10)	−0.0049 (11)
N4	0.0144 (12)	0.0152 (13)	0.0163 (13)	−0.0040 (11)	0.0003 (10)	−0.0048 (11)
C2	0.0146 (15)	0.0147 (16)	0.0221 (16)	−0.0056 (12)	0.0029 (12)	−0.0080 (13)
C1	0.0154 (15)	0.0176 (17)	0.0361 (19)	−0.0064 (13)	0.0028 (14)	−0.0063 (15)
C3	0.0213 (16)	0.0181 (16)	0.0218 (16)	−0.0137 (14)	0.0056 (13)	−0.0054 (13)
C4	0.0185 (15)	0.0122 (15)	0.0137 (14)	−0.0072 (13)	0.0013 (12)	−0.0040 (12)
C5	0.0207 (16)	0.0095 (15)	0.0251 (17)	−0.0030 (13)	0.0013 (13)	−0.0037 (13)
C9	0.0188 (15)	0.0168 (16)	0.0219 (16)	−0.0110 (13)	0.0035 (13)	−0.0040 (13)

C10	0.0208 (16)	0.0145 (16)	0.0264 (17)	−0.0030 (13)	−0.0009 (13)	−0.0036 (14)
C8	0.0175 (16)	0.0168 (16)	0.0169 (15)	−0.0047 (13)	−0.0010 (12)	−0.0013 (13)
C7	0.0188 (15)	0.0166 (16)	0.0182 (16)	−0.0097 (13)	0.0026 (12)	−0.0051 (13)
C6	0.0222 (17)	0.0233 (18)	0.0237 (17)	−0.0061 (14)	0.0024 (14)	−0.0094 (14)
C11	0.0139 (14)	0.0128 (15)	0.0203 (15)	−0.0062 (12)	0.0036 (12)	−0.0087 (13)
C12	0.0171 (15)	0.0197 (17)	0.0175 (16)	−0.0092 (13)	0.0025 (12)	−0.0066 (13)

Geometric parameters (Å, º)

Cu1—O2	1.946 (2)	C1—H4	0.9800
Cu1—O5	1.971 (2)	C1—H6	0.9800
Cu1—N2	1.975 (3)	C1—H5	0.9800
Cu1—N3	2.002 (2)	C3—C4	1.390 (4)
Cu1—O1	2.283 (2)	C3—H7	0.9500
O5—C12	1.285 (4)	C4—C5	1.503 (4)
O2—C11	1.261 (4)	C5—H10	0.9800
O4—C12	1.225 (4)	C5—H8	0.9800
O3—C11	1.256 (4)	C5—H9	0.9800
O1—H1	0.9902	C9—C8	1.367 (5)
O1—H2	0.9664	C9—C10	1.497 (4)
N2—C4	1.341 (4)	C10—H15	0.9800
N2—N1	1.359 (3)	C10—H16	0.9800
N1—C2	1.345 (4)	C10—H17	0.9800
N1—H3	0.8800	C8—C7	1.408 (4)
N3—C7	1.337 (4)	C8—H14	0.9500
N3—N4	1.355 (3)	C7—C6	1.487 (4)
N4—C9	1.352 (4)	C6—H12	0.9800
N4—H18	0.8800	C6—H13	0.9800
C2—C3	1.383 (4)	C6—H11	0.9800
C2—C1	1.490 (4)	C11—C12	1.561 (4)
O2—Cu1—O5	84.54 (9)	C4—C3—H7	126.9
O2—Cu1—N2	172.35 (10)	N2—C4—C3	110.0 (3)
O5—Cu1—N2	92.59 (9)	N2—C4—C5	122.3 (3)
O2—Cu1—N3	88.41 (10)	C3—C4—C5	127.7 (3)
O5—Cu1—N3	170.11 (10)	C4—C5—H10	109.5
N2—Cu1—N3	93.53 (10)	C4—C5—H8	109.5
O2—Cu1—O1	89.05 (9)	H10—C5—H8	109.5
O5—Cu1—O1	91.85 (9)	C4—C5—H9	109.5
N2—Cu1—O1	98.15 (10)	H10—C5—H9	109.5
N3—Cu1—O1	94.96 (9)	H8—C5—H9	109.5
C12—O5—Cu1	112.55 (18)	N4—C9—C8	106.8 (3)
C11—O2—Cu1	112.86 (18)	N4—C9—C10	120.6 (3)
Cu1—O1—H1	115.9	C8—C9—C10	132.6 (3)
Cu1—O1—H2	130.8	C9—C10—H15	109.5
H1—O1—H2	111.5	C9—C10—H16	109.5
C4—N2—N1	105.8 (2)	H15—C10—H16	109.5
C4—N2—Cu1	132.3 (2)	C9—C10—H17	109.5

N1—N2—Cu1	121.3 (2)	H15—C10—H17	109.5
C2—N1—N2	111.5 (3)	H16—C10—H17	109.5
C2—N1—H3	124.2	C9—C8—C7	106.3 (3)
N2—N1—H3	124.2	C9—C8—H14	126.9
C7—N3—N4	106.3 (2)	C7—C8—H14	126.9
C7—N3—Cu1	133.1 (2)	N3—C7—C8	109.3 (3)
N4—N3—Cu1	120.31 (19)	N3—C7—C6	121.3 (3)
C9—N4—N3	111.3 (3)	C8—C7—C6	129.3 (3)
C9—N4—H18	124.4	C7—C6—H12	109.5
N3—N4—H18	124.4	C7—C6—H13	109.5
N1—C2—C3	106.5 (3)	H12—C6—H13	109.5
N1—C2—C1	122.5 (3)	C7—C6—H11	109.5
C3—C2—C1	131.0 (3)	H12—C6—H11	109.5
C2—C1—H4	109.5	H13—C6—H11	109.5
C2—C1—H6	109.5	O3—C11—O2	125.0 (3)
H4—C1—H6	109.5	O3—C11—C12	118.7 (3)
C2—C1—H5	109.5	O2—C11—C12	116.2 (3)
H4—C1—H5	109.5	O4—C12—O5	127.2 (3)
H6—C1—H5	109.5	O4—C12—C11	119.0 (3)
C2—C3—C4	106.2 (3)	O5—C12—C11	113.7 (3)
C2—C3—H7	126.9		

O2—Cu1—O5—C12	−3.4 (2)	C1—C2—C3—C4	179.7 (3)
N2—Cu1—O5—C12	169.5 (2)	N1—N2—C4—C3	−0.5 (3)
O1—Cu1—O5—C12	−92.3 (2)	Cu1—N2—C4—C3	−171.4 (2)
O5—Cu1—O2—C11	3.0 (2)	N1—N2—C4—C5	−179.4 (3)
N3—Cu1—O2—C11	−170.0 (2)	Cu1—N2—C4—C5	9.7 (5)
O1—Cu1—O2—C11	95.0 (2)	C2—C3—C4—N2	−0.1 (4)
O5—Cu1—N2—C4	134.5 (3)	C2—C3—C4—C5	178.7 (3)
N3—Cu1—N2—C4	−53.3 (3)	N3—N4—C9—C8	0.2 (4)
O1—Cu1—N2—C4	42.2 (3)	N3—N4—C9—C10	−179.6 (3)
O5—Cu1—N2—N1	−35.3 (2)	N4—C9—C8—C7	−0.2 (4)
N3—Cu1—N2—N1	137.0 (2)	C10—C9—C8—C7	179.5 (3)
O1—Cu1—N2—N1	−127.5 (2)	N4—N3—C7—C8	0.0 (3)
C4—N2—N1—C2	0.9 (3)	Cu1—N3—C7—C8	173.5 (2)
Cu1—N2—N1—C2	173.1 (2)	N4—N3—C7—C6	−179.8 (3)
O2—Cu1—N3—C7	123.6 (3)	Cu1—N3—C7—C6	−6.2 (5)
N2—Cu1—N3—C7	−49.0 (3)	C9—C8—C7—N3	0.1 (4)
O1—Cu1—N3—C7	−147.5 (3)	C9—C8—C7—C6	179.9 (3)
O2—Cu1—N3—N4	−63.5 (2)	Cu1—O2—C11—O3	175.7 (2)
N2—Cu1—N3—N4	123.9 (2)	Cu1—O2—C11—C12	−2.2 (3)
O1—Cu1—N3—N4	25.4 (2)	Cu1—O5—C12—O4	−176.5 (3)
C7—N3—N4—C9	−0.1 (3)	Cu1—O5—C12—C11	3.1 (3)
Cu1—N3—N4—C9	−174.7 (2)	O3—C11—C12—O4	1.0 (4)
N2—N1—C2—C3	−1.0 (4)	O2—C11—C12—O4	179.0 (3)
N2—N1—C2—C1	179.8 (3)	O3—C11—C12—O5	−178.6 (3)
N1—C2—C3—C4	0.7 (3)	O2—C11—C12—O5	−0.6 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{i}	0.99	1.88	2.798 (3)	153
O1—H2···O5^{ii}	0.97	1.97	2.923 (3)	168
N1—H3···O3^{iii}	0.88	2.03	2.857 (3)	156
N4—H18···O3^{i}	0.88	1.97	2.845 (3)	175

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