Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetra-μ-acetato-κ^8O:O'-bis{[2,2-dimethyl-*N*-(pyridin-2-yl)propanamide-κN^1]-copper(II)}(*Cu*—*Cu*)

Samuel Asem, Robert M. Buchanan and Mark S. Mashuta*

Department of Chemistry, University of Louisville, Louisville, KY 40292, USA
Correspondence e-mail: msmashuta.xray@louisville.edu

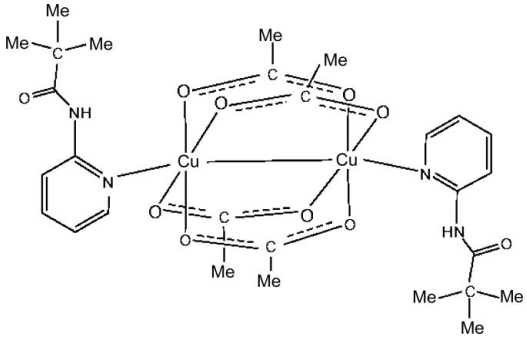
Received 8 November 2011; accepted 22 November 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.094; data-to-parameter ratio = 16.9.

The crystal structure of the title compound, $[Cu_2(C_2H_3O_2)_4(C_{10}H_{14}N_2O)_2]$, reveals a dinuclear Cu^{II} complex located about a center of inversion. The coordination environment of each Cu^{II} cation is distorted octahedral, composed of four bridging acetate ligands, an apical pyridine donor and is completed by a Cu—Cu bond. The amide H atom forms intramolecular hydrogen bonds to two carboxyl O atoms. In the crystal, weak intermolecular pyridine–amide C—H···O interactions are also present.

Related literature

For related paddlewheel structures, see: Aakeröy *et al.* (2003); Barquín *et al.* (2004, 2006); Fairuz *et al.* (2010); Seco *et al.* (2004); Sieroń (2004); Shi *et al.* (2008). For Cu···Cu separations in related compounds, see: Seco *et al.* (2004). For hydrogen bonding, see: Desiraju (1995).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{10}H_{14}N_2O)_2]$
M_r = 719.74
Monoclinic, $P2_1/c$
a = 13.8508 (8) Å
b = 11.0612 (5) Å
c = 11.0301 (6) Å
β = 104.508 (6)°
V = 1635.98 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.36 mm^{-1}
T = 100 K
0.41 × 0.38 × 0.38 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.581, T_{max} = 0.602
7567 measured reflections
3515 independent reflections
3070 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.01
3515 reflections
208 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O3	1.9670 (17)	Cu1—O1	1.9762 (16)
Cu1—O2	1.9734 (17)	Cu1—N1	2.1990 (19)
Cu1—O4	1.9739 (16)	Cu1—Cu1^{i}	2.6168 (6)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···O4	0.80	2.38	3.118 (3)	154.1
N2—H2*N*···O2	0.80	2.71	3.226 (3)	124.0
C7—H7···O5^{ii}	0.95	2.69	3.298 (3)	122
C8—H8···O5^{ii}	0.95	2.63	3.262 (3)	124
C6—H6···O1^{iii}	0.95	2.58	3.460 (3)	154

Symmetry codes: (ii) $-x+2, -y+1, -z+2$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

MSM thanks the Department of Energy, grant DEFG02–08CH11538, and the Kentucky Research Challenge Trust Fund for the upgrade of our X-ray facilities. SA thanks the University of Louisville for graduate student minority fellowship support. RMB thanks the Kentucky Science and Engineering Foundation (grant KSEF-275-RDE-003) for financial support of this research.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5186).

References

Aakeröy, C. B., Beatty, A. M., Desper, J., O'Shea, M. & Valdés-Martínez, J. (2003). *Dalton Trans.* pp. 3956–3962.
Barquín, M., González Garmendia, M. J., Larrínaga, L., Pinilla, E. & Torres, M. R. (2006). *Inorg. Chim. Acta*, **359**, 2424-2430.
Barquín, M., González Garmendia, M. J., Pachecco, S., Pinilla, E., Quintela, S., Seco, J. M. & Torres, M. R. (2004). *Inorg. Chim. Acta*, **357**, 3230–3236.

Desiraju, G. R. (1995). *Angew. Chem. Int. Ed.* **34**, 2311–2327.
Fairuz, Z. A., Aiyub, Z., Abdullah, Z., Ng, S. W. & Tiekink, E. R. T. (2010). *Acta Cryst.* E**66**, m1049–m1050.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Oxford Diffraction (2009). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Seco, J. M., González Garmendia, M. J., Pinilla, E. & Torres, M. R. (2004). *Polyhedron*, **21**, 457–464.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shi, C.-Y., Ge, C.-H., Gao, E.-J., Yin, H.-X. & Lui, Q.-T. (2008). *Inorg. Chem. Commun.* **11**, 703–706.
Sieroń, L. (2004). *Acta Cryst.* E**60**, m577–m578.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2011). E**67**, m1892-m1893 [**doi:10.1107/S1600536811050124**]

Tetra-μ-acetato-$\kappa^8O:O'$-bis{[2,2-dimethyl-*N*-(pyridin-2-yl)propanamide-κN^1]copper(II)}(*Cu*-*Cu*)

S. Asem, R. M. Buchanan and M. S. Mashuta

Comment

Amide functionalized pyridine ligands have the potential to be used in the synthesis of supramolecular materials; particularly transition metal coordination polymers. The title complex, (I), is structurally similar to paddlewheel structures of other $Cu_2(OAc)_4L_2$ complexes. (Aakeröy *et al.*, 2003; Barquín *et al.*, 2004, 2006; Fairuz *et al.*, 2010; Seco *et al.*; 2004; Sieroń, 2004; Shi, *et al.*, 2008). The dinuclear molecule lies about an inversion center. Attached to this $Cu_2(OAc)_4$ core unit are two apical pyridine ligands functionalized in the 2-position of the ring with a pendant amide. The average Cu-O (1.9726 (17) Å) and Cu-N (2.1990 (19) Å) distances and corresponding bond angles are consistent with structurally similar Cu^{II} complexes (Table 1). While the Cu—Cu separation of 2.6168 (6) Å) is towards the lower limit, it is within the range of values reported for Cu^{II} paddlewheel structures. (Sieroń, 2004). The amide hydrogen forms intramolecular hydrogen bonds to two acetate oxygen atoms N2-H2- - -O4 and N2-H2- - -O2 (Table 2), (Desiraju, 1995). There are also three weak intermolecular C_{py}-H- - -O amide interactions between adjacent metal complexes, C7-H7- - -O5, C8-H8- - -O5 and C6-H6- - -O1 (Table 2). These interactions result in the formation of infinite linear chains along the crystallographic AC diagonal and project through the BC face. The amide group and pyridine ring display a twist angle (C9-NH2-C10-O5) of 3.3 (4)°.

Experimental

A stirred solution of (2-pivaloylamino)pyridine (0.4150 g, 2.328 mmol) in acetone (10 ml) was combined with a solution of $Cu(CH_3COO)_2H_2O$ (0.2324 g, 1.1642 mmol) in methanol (20 ml). The reaction was refluxed for an hour and stirring was continued for 24 h at room temperature. The reaction mixture was filtered and the solvent was removed *via* rotary evaporation. The resulting solid was dissolved in diethyl ether from which blue-green crystals deposited over several days.

Refinement

The amide hydrogen atom was located from difference maps and refined isotropically. Aromatic H atom positions were calculated, and included as fixed contributions with U_{iso}(H) = 1.2 *x* U_{eq}(C). Methyl H atoms were placed in calculated positions and allowed to ride (the torsion angle which defines its orientation was allowed to refine) on the attached C atom, and these atoms were assigned U_{iso}(H) = 1.5 *x* U_{eq}(C). The highest peak, 0.73 e/Å^3, and deepest trough, -0.58 e/Å^3, are located 1.10 Å and 0.82 Å from Cu1 respectively.

Figures

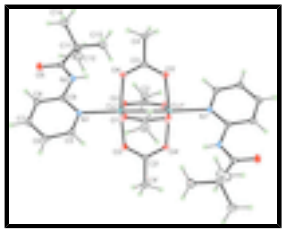


Fig. 1. *ORTEP-3* (Farrugia, 1997) view of (I) showing 50% displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

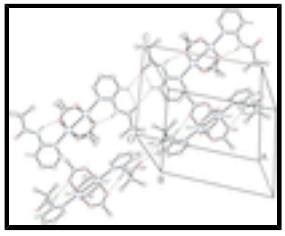


Fig. 2. Packing diagram displaying hydrogen-bonding interactions. [Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z* + 1 (ii) -*x*+2, 1 - *y*, -*z*] (iii) *x*, -*y* + 3/2, *z* + 1/2.

Tetra-μ-acetato-κ^8*O*:*O*'-bis{[2,2-dimethyl-*N*- (pyridin-2-yl)propanamide-κ*N*^{1}]copper(II)}(*Cu*—*Cu*)

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{10}H_{14}N_2O)_2]$	$F(000) = 748$
$M_r = 719.74$	$D_x = 1.461$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4128 reflections
$a = 13.8508$ (8) Å	$\theta = 3.6$–$28.8°$
$b = 11.0612$ (5) Å	$\mu = 1.36$ mm^{-1}
$c = 11.0301$ (6) Å	$T = 100$ K
$\beta = 104.508$ (6)°	Block, blue-green
$V = 1635.98$ (15) Å^3	0.41 × 0.38 × 0.38 mm
$Z = 2$	

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer	3515 independent reflections
Radiation source: Enhance (Mo) X-ray Source	3070 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.032$
Detector resolution: 10.2836 pixels mm^{-1}	$\theta_{max} = 27.1°$, $\theta_{min} = 3.6°$
ω scans	$h = -17 \rightarrow 10$
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)	$k = -11 \rightarrow 13$
$T_{min} = 0.581$, $T_{max} = 0.602$	$l = -13 \rightarrow 14$
7567 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.094$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 1.875P]$ where $P = (F_o^2 + 2F_c^2)/3$
3515 reflections	$(\Delta/\sigma)_{max} = 0.001$
208 parameters	$\Delta\rho_{max} = 0.73$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.58$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.57135 (2)	0.51365 (2)	0.60219 (2)	0.01145 (10)
O1	0.52507 (13)	0.68323 (15)	0.58335 (15)	0.0168 (4)
O2	0.59958 (13)	0.33989 (15)	0.58943 (15)	0.0193 (4)
O3	0.46567 (13)	0.47616 (16)	0.68677 (15)	0.0186 (4)
O4	0.65766 (12)	0.54422 (16)	0.48765 (15)	0.0163 (4)
O5	0.96072 (13)	0.38557 (17)	0.84694 (16)	0.0238 (4)
N1	0.68384 (14)	0.55679 (18)	0.77605 (17)	0.0136 (4)
N2	0.81361 (16)	0.4539 (2)	0.7259 (2)	0.0182 (4)
H2N	0.778 (2)	0.455 (3)	0.657 (3)	0.017 (7)*
C1	0.54803 (18)	0.2779 (2)	0.4997 (2)	0.0148 (5)
C2	0.5762 (2)	0.1471 (2)	0.4927 (2)	0.0233 (6)
H2A	0.5555	0.1020	0.5562	0.035*
H2B	0.6472	0.1406	0.5056	0.035*
H2C	0.5438	0.1153	0.4117	0.035*
C3	0.62383 (18)	0.5437 (2)	0.3700 (2)	0.0144 (5)
C4	0.6955 (2)	0.5688 (3)	0.2908 (2)	0.0229 (6)
H4A	0.7117	0.4945	0.2555	0.034*
H4B	0.7552	0.6044	0.3417	0.034*
H4C	0.6653	0.6236	0.2247	0.034*
C5	0.64649 (18)	0.6255 (2)	0.8544 (2)	0.0158 (5)
H5	0.5800	0.6491	0.8289	0.019*
C6	0.70168 (19)	0.6627 (2)	0.9702 (2)	0.0167 (5)
H6	0.6730	0.7087	1.0225	0.020*
C7	0.80085 (19)	0.6297 (2)	1.0061 (2)	0.0181 (5)
H7	0.8404	0.6546	1.0832	0.022*
C8	0.84148 (18)	0.5597 (2)	0.9276 (2)	0.0175 (5)
H8	0.9082	0.5369	0.9508	0.021*
C9	0.78030 (18)	0.5243 (2)	0.8134 (2)	0.0143 (5)
C10	0.89929 (18)	0.3871 (2)	0.7467 (2)	0.0155 (5)

C11	0.91516 (19)	0.3108 (2)	0.6368 (2)	0.0190 (5)
C12	0.9151 (3)	0.1789 (3)	0.6784 (3)	0.0431 (9)
H12A	0.8508	0.1587	0.6904	0.065*
H12B	0.9649	0.1678	0.7556	0.065*
H12C	0.9297	0.1274	0.6152	0.065*
C13	0.8377 (2)	0.3303 (3)	0.5133 (3)	0.0352 (7)
H13A	0.7731	0.3073	0.5225	0.053*
H13B	0.8544	0.2818	0.4493	0.053*
H13C	0.8368	0.4140	0.4902	0.053*
C14	1.0181 (2)	0.3433 (3)	0.6186 (3)	0.0328 (7)
H14A	1.0300	0.2981	0.5495	0.049*
H14B	1.0683	0.3239	0.6933	0.049*
H14C	1.0205	0.4282	0.6016	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01005 (16)	0.01279 (16)	0.01139 (16)	−0.00018 (11)	0.00250 (11)	−0.00009 (10)
O1	0.0154 (9)	0.0141 (8)	0.0198 (8)	0.0014 (7)	0.0025 (7)	−0.0011 (7)
O2	0.0190 (9)	0.0137 (8)	0.0222 (9)	0.0005 (7)	−0.0001 (7)	−0.0003 (7)
O3	0.0151 (9)	0.0253 (9)	0.0157 (8)	−0.0057 (7)	0.0046 (7)	0.0015 (7)
O4	0.0120 (8)	0.0230 (9)	0.0143 (8)	−0.0022 (7)	0.0040 (6)	0.0002 (7)
O5	0.0192 (9)	0.0297 (10)	0.0197 (9)	0.0091 (8)	−0.0006 (7)	−0.0054 (8)
N1	0.0120 (10)	0.0161 (10)	0.0133 (9)	0.0000 (8)	0.0042 (8)	−0.0010 (8)
N2	0.0124 (10)	0.0269 (12)	0.0137 (10)	0.0030 (9)	0.0003 (8)	−0.0074 (9)
C1	0.0143 (12)	0.0145 (11)	0.0170 (11)	0.0002 (9)	0.0067 (9)	0.0016 (9)
C2	0.0224 (14)	0.0155 (12)	0.0295 (14)	0.0029 (11)	0.0019 (11)	−0.0008 (10)
C3	0.0161 (12)	0.0112 (11)	0.0173 (11)	0.0011 (9)	0.0066 (9)	0.0006 (9)
C4	0.0197 (13)	0.0325 (15)	0.0190 (12)	−0.0029 (11)	0.0097 (10)	0.0022 (11)
C5	0.0142 (12)	0.0165 (12)	0.0169 (11)	0.0029 (9)	0.0045 (9)	0.0000 (9)
C6	0.0215 (13)	0.0159 (11)	0.0140 (11)	0.0031 (10)	0.0070 (10)	−0.0014 (9)
C7	0.0196 (13)	0.0189 (12)	0.0135 (11)	0.0011 (10)	−0.0002 (9)	−0.0034 (9)
C8	0.0132 (12)	0.0214 (12)	0.0166 (11)	0.0017 (10)	0.0016 (9)	−0.0021 (10)
C9	0.0147 (12)	0.0153 (11)	0.0133 (11)	0.0005 (9)	0.0040 (9)	−0.0007 (9)
C10	0.0131 (12)	0.0163 (12)	0.0177 (11)	−0.0012 (9)	0.0048 (9)	−0.0010 (9)
C11	0.0151 (12)	0.0231 (13)	0.0194 (12)	0.0038 (10)	0.0055 (10)	−0.0049 (10)
C12	0.073 (3)	0.0217 (15)	0.0434 (18)	−0.0007 (16)	0.0299 (18)	−0.0092 (14)
C13	0.0234 (15)	0.057 (2)	0.0236 (13)	0.0121 (14)	0.0026 (12)	−0.0191 (14)
C14	0.0220 (15)	0.0509 (19)	0.0284 (14)	0.0001 (14)	0.0116 (12)	−0.0073 (14)

Geometric parameters (Å, °)

Cu1—O3	1.9670 (17)	C4—H4C	0.9600
Cu1—O2	1.9734 (17)	C5—C6	1.377 (3)
Cu1—O4	1.9739 (16)	C5—H5	0.9300
Cu1—O1	1.9762 (16)	C6—C7	1.380 (3)
Cu1—N1	2.1990 (19)	C6—H6	0.9300
Cu1—Cu1^{i}	2.6168 (6)	C7—C8	1.382 (3)

O1—C1^{i}	1.259 (3)	C7—H7	0.9300
O2—C1	1.267 (3)	C8—C9	1.387 (3)
O3—C3^{i}	1.260 (3)	C8—H8	0.9300
O4—C3	1.264 (3)	C10—C11	1.537 (3)
O5—C10	1.215 (3)	C11—C13	1.524 (4)
N1—C9	1.345 (3)	C11—C12	1.529 (4)
N1—C5	1.348 (3)	C11—C14	1.532 (4)
N2—C10	1.368 (3)	C12—H12A	0.9600
N2—C9	1.405 (3)	C12—H12B	0.9600
N2—H2N	0.79 (3)	C12—H12C	0.9600
C1—C2	1.506 (3)	C13—H13A	0.9600
C2—H2A	0.9600	C13—H13B	0.9600
C2—H2B	0.9600	C13—H13C	0.9600
C2—H2C	0.9600	C14—H14A	0.9600
C3—C4	1.503 (3)	C14—H14B	0.9600
C4—H4A	0.9600	C14—H14C	0.9600
C4—H4B	0.9600		
O3—Cu1—O2	90.73 (8)	N1—C5—C6	123.4 (2)
O3—Cu1—O4	169.00 (7)	N1—C5—H5	118.3
O2—Cu1—O4	87.63 (8)	C6—C5—H5	118.3
O3—Cu1—O1	89.41 (7)	C5—C6—C7	118.0 (2)
O2—Cu1—O1	169.03 (7)	C5—C6—H6	121.0
O4—Cu1—O1	90.15 (7)	C7—C6—H6	121.0
O3—Cu1—N1	94.65 (7)	C6—C7—C8	120.0 (2)
O2—Cu1—N1	99.43 (7)	C6—C7—H7	120.0
O4—Cu1—N1	96.35 (7)	C8—C7—H7	120.0
O1—Cu1—N1	91.49 (7)	C7—C8—C9	118.4 (2)
O3—Cu1—Cu1^{i}	83.86 (5)	C7—C8—H8	120.8
O2—Cu1—Cu1^{i}	86.93 (5)	C9—C8—H8	120.8
O4—Cu1—Cu1^{i}	85.19 (5)	N1—C9—C8	122.5 (2)
O1—Cu1—Cu1^{i}	82.18 (5)	N1—C9—N2	114.2 (2)
N1—Cu1—Cu1^{i}	173.50 (6)	C8—C9—N2	123.3 (2)
C1^{i}—O1—Cu1	125.55 (15)	O5—C10—N2	122.7 (2)
C1—O2—Cu1	119.99 (15)	O5—C10—C11	120.3 (2)
C3^{i}—O3—Cu1	123.85 (15)	N2—C10—C11	117.0 (2)
C3—O4—Cu1	121.86 (15)	C13—C11—C12	110.5 (3)
C9—N1—C5	117.8 (2)	C13—C11—C14	108.6 (2)
C9—N1—Cu1	129.93 (15)	C12—C11—C14	109.5 (3)
C5—N1—Cu1	112.31 (15)	C13—C11—C10	114.8 (2)
C10—N2—C9	127.2 (2)	C12—C11—C10	106.1 (2)
C10—N2—H2N	118 (2)	C14—C11—C10	107.2 (2)
C9—N2—H2N	115 (2)	C11—C12—H12A	109.5
O1^{i}—C1—O2	125.2 (2)	C11—C12—H12B	109.5
O1^{i}—C1—C2	117.5 (2)	H12A—C12—H12B	109.5
O2—C1—C2	117.2 (2)	C11—C12—H12C	109.5
C1—C2—H2A	109.5	H12A—C12—H12C	109.5

C1—C2—H2B	109.5	H12B—C12—H12C	109.5
H2A—C2—H2B	109.5	C11—C13—H13A	109.5
C1—C2—H2C	109.5	C11—C13—H13B	109.5
H2A—C2—H2C	109.5	H13A—C13—H13B	109.5
H2B—C2—H2C	109.5	C11—C13—H13C	109.5
$O3^{i}$—C3—O4	125.2 (2)	H13A—C13—H13C	109.5
$O3^{i}$—C3—C4	117.0 (2)	H13B—C13—H13C	109.5
O4—C3—C4	117.8 (2)	C11—C14—H14A	109.5
C3—C4—H4A	109.5	C11—C14—H14B	109.5
C3—C4—H4B	109.5	H14A—C14—H14B	109.5
H4A—C4—H4B	109.5	C11—C14—H14C	109.5
C3—C4—H4C	109.5	H14A—C14—H14C	109.5
H4A—C4—H4C	109.5	H14B—C14—H14C	109.5
H4B—C4—H4C	109.5		
O3—Cu1—O1—$C1^{i}$	−80.42 (19)	O1—Cu1—N1—C5	45.82 (17)
O2—Cu1—O1—$C1^{i}$	10.4 (5)	Cu1—O2—C1—$O1^{i}$	−2.9 (3)
O4—Cu1—O1—$C1^{i}$	88.59 (19)	Cu1—O2—C1—C2	177.59 (16)
N1—Cu1—O1—$C1^{i}$	−175.05 (19)	Cu1—O4—C3—$O3^{i}$	−0.3 (3)
$Cu1^{i}$—Cu1—O1—$C1^{i}$	3.46 (18)	Cu1—O4—C3—C4	179.58 (17)
O3—Cu1—O2—C1	84.00 (18)	C9—N1—C5—C6	−0.6 (4)
O4—Cu1—O2—C1	−85.12 (18)	Cu1—N1—C5—C6	178.83 (19)
O1—Cu1—O2—C1	−6.7 (5)	N1—C5—C6—C7	1.4 (4)
N1—Cu1—O2—C1	178.83 (17)	C5—C6—C7—C8	−1.0 (4)
$Cu1^{i}$—Cu1—O2—C1	0.19 (17)	C6—C7—C8—C9	0.0 (4)
O2—Cu1—O3—$C3^{i}$	−88.33 (19)	C5—N1—C9—C8	−0.6 (3)
O4—Cu1—O3—$C3^{i}$	−7.0 (5)	Cu1—N1—C9—C8	−179.89 (18)
O1—Cu1—O3—$C3^{i}$	80.70 (19)	C5—N1—C9—N2	−179.3 (2)
N1—Cu1—O3—$C3^{i}$	172.15 (19)	Cu1—N1—C9—N2	1.3 (3)
$Cu1^{i}$—Cu1—O3—$C3^{i}$	−1.49 (18)	C7—C8—C9—N1	0.9 (4)
O3—Cu1—O4—C3	6.6 (5)	C7—C8—C9—N2	179.6 (2)
O2—Cu1—O4—C3	88.17 (18)	C10—N2—C9—N1	−165.0 (2)
O1—Cu1—O4—C3	−81.08 (18)	C10—N2—C9—C8	16.2 (4)
N1—Cu1—O4—C3	−172.60 (18)	C9—N2—C10—O5	−3.3 (4)
$Cu1^{i}$—Cu1—O4—C3	1.05 (17)	C9—N2—C10—C11	175.9 (2)
O3—Cu1—N1—C9	135.7 (2)	O5—C10—C11—C13	−174.4 (3)
O2—Cu1—N1—C9	44.1 (2)	N2—C10—C11—C13	6.4 (3)
O4—Cu1—N1—C9	−44.5 (2)	O5—C10—C11—C12	63.3 (3)
O1—Cu1—N1—C9	−134.8 (2)	N2—C10—C11—C12	−115.9 (3)
O3—Cu1—N1—C5	−43.71 (17)	O5—C10—C11—C14	−53.6 (3)
O2—Cu1—N1—C5	−135.22 (16)	N2—C10—C11—C14	127.2 (2)
O4—Cu1—N1—C5	136.14 (16)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2N···O4	0.80	2.38	3.118 (3)	154.1
N2—H2N···O2	0.80	2.71	3.226 (3)	124.0
C7—H7···O5^{ii}	0.95	2.69	3.298 (3)	122.
C8—H8···O5^{ii}	0.95	2.63	3.262 (3)	124.
C6—H6···O1^{iii}	0.95	2.58	3.460 (3)	154

Symmetry codes: (ii) −*x*+2, −*y*+1, −*z*+2; (iii) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

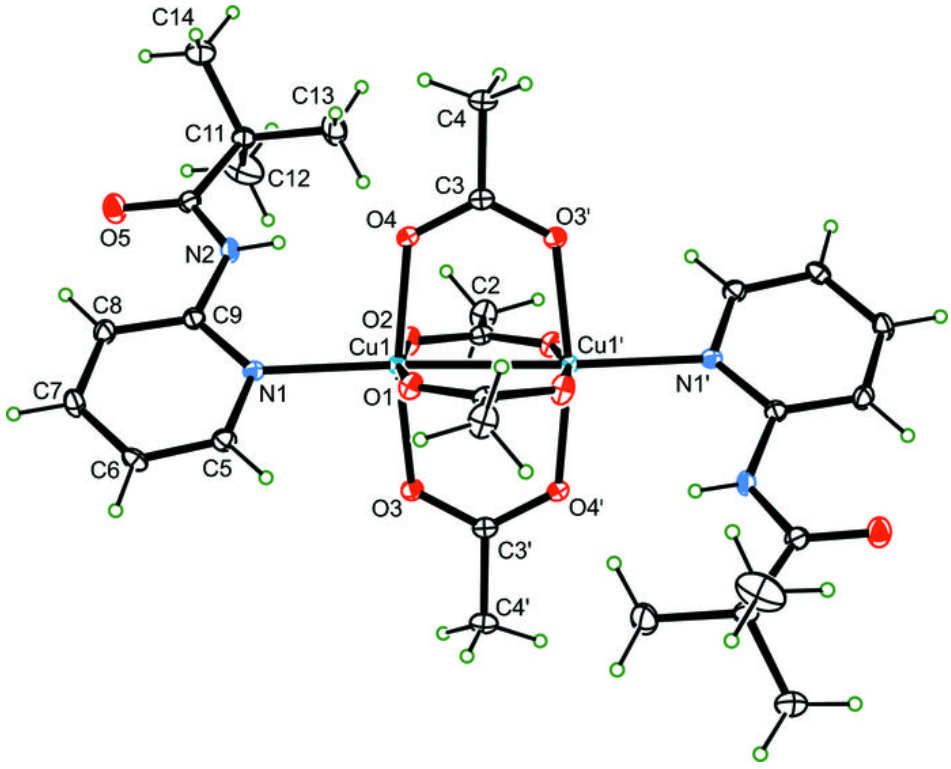

C14
C13
C11
C12
C4
C3
O5
N2
O4
O3'
C2
C8
C9
O2
Cu1
Cu1'
C7
N1
O1
N1'
C6
C5
O3
O4'
C3'
C4'

Fig. 2