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Aquabis(dichloroacetato- κ O)(1,10-phenanthroline- κ^2 N,N')copper(II)

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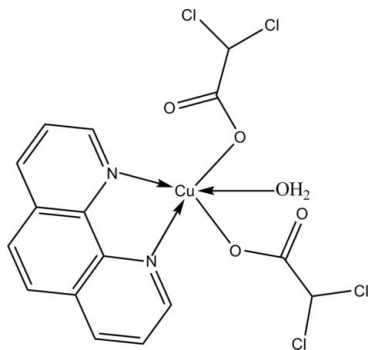
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 Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.042; wR factor = 0.106; data-to-parameter ratio = 12.8.

In the title complex, $[\text{Cu}(\text{C}_2\text{HCl}_2\text{O}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$, the Cu^{II} ion has a distorted square-pyramidal coordination geometry. The equatorial positions are occupied by two N atoms from a 1,10-phenanthroline ligand [$\text{Cu}-\text{N} = 1.994$ (3) and 2.027 (3) Å] and two O atoms from dichloroacetate ligands and a water molecule [$\text{Cu}-\text{O} = 1.971$ (2) and 1.939 (2) Å]. One O atom from another dichloroacetate ligand occupies the apical position [$\text{Cu}-\text{O} = 2.152$ (3) Å]. Intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into centrosymmetric dimers. The crystal packing also exhibits weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, $\pi-\pi$ interactions [centroid-centroid distance = 3.734 (2) Å] and short intermolecular $\text{Cl}\cdots\text{Cl}$ contacts [3.306 (2) and 3.278 (2) Å].

Related literature

 For applications of dichloroacetic acid derivatives, see: Múdra *et al.* (2003); Lin *et al.* (2001); Zhu & Xiao (2006).


Experimental

Crystal data

$[\text{Cu}(\text{C}_2\text{HCl}_2\text{O}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$
 $M_r = 517.62$
 Triclinic, $P\bar{1}$
 $a = 8.2701$ (8) Å
 $b = 10.8883$ (11) Å
 $c = 12.0125$ (12) Å
 $\alpha = 67.4390$ (10)°
 $\beta = 77.585$ (2)°
 $\gamma = 73.776$ (2)°
 $V = 952.02$ (16) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.74$ mm⁻¹
 $T = 273$ (2) K
 $0.32 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.606$, $T_{\text{max}} = 0.711$
 5043 measured reflections
 3346 independent reflections
 2539 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.106$
 $S = 1.01$
 3346 reflections
 261 parameters
 3 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.51$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C16}-\text{H16}\cdots\text{O2}^{\text{i}}$	0.98	2.24	3.118 (5)	149
$\text{O5}-\text{H5B}\cdots\text{O2}^{\text{ii}}$	0.85 (2)	1.81 (2)	2.654 (3)	174 (3)
$\text{O5}-\text{H5A}\cdots\text{O4}$	0.85 (2)	1.86 (2)	2.673 (4)	159 (3)

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; 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: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2493).

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supporting information

Acta Cryst. (2009). E65, m113 [doi:10.1107/S1600536808042578]

Aquabis(dichloroacetato- κ O)(1,10-phenanthroline- κ^2 N,N')copper(II)

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S1. Comment

Dichloroacetic acid and its derivatives are biologically active compounds which have been widely studied because of their fascinating topologies and potential applications as functional materials (Múdra *et al.*, 2003; Lin *et al.*, 2001; Zhu *et al.*, 2006;). In our study of this field, we selected 1,10-phenanthroline as the co-ligand to continue our exploration to the Cu complexes with the dichloroacetic acid ligand. Herein we report the structure of the title complex (I).

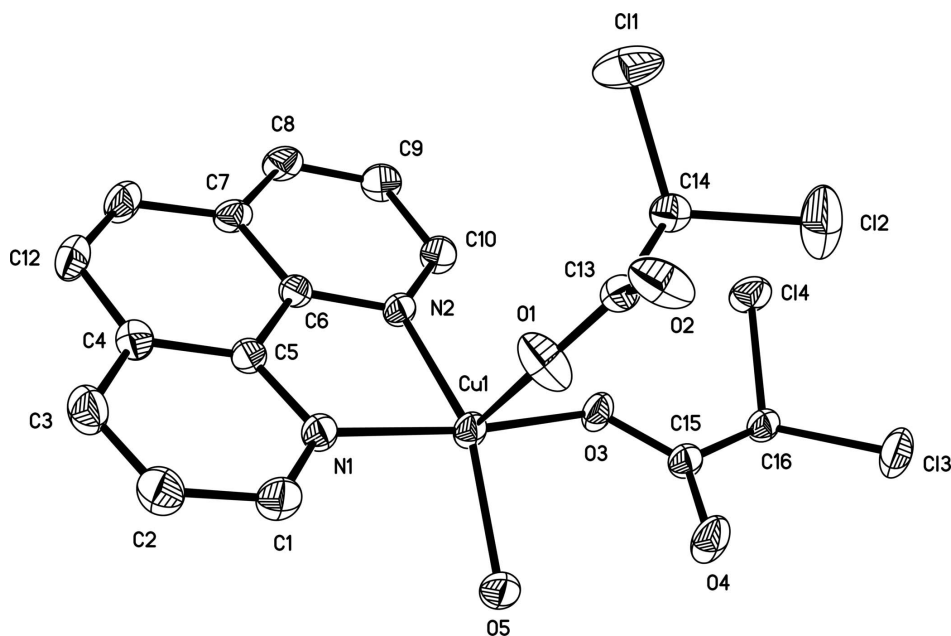
In (I) (Fig. 1), the Cu ion has a distorted square-pyramidal coordination. Two N atoms from 1,10-phenanthroline ligand and two oxygen atoms from a dichloroacetic acid ligand form a basal plane, and an aqua atom occupy the axial apical position. Intermolecular O—H \cdots O hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers. The crystal packing exhibits also weak intermolecular C—H \cdots O hydrogen bonds, π – π interactions and short intermolecular Cl \cdots Cl contacts (Table 1).

S2. Experimental

A mixture of Cu(CH₃COO)₂·3H₂O (204 mg, 1 mmol) and 1,10-phenanthroline (185 mg, 1 mmol) in methanol (30 ml) was placed in a Teflon-lined stainless steel Parr bomb that was heated at 403 K for 48 h. The bomb was then cooled down to the room temperature, the solution was filtered. The solvent was removed from the filtrate under vacuum, and the solid residue was recrystallized from diethyl ether; blue crystals suitable for X-Ray diffraction study were obtained. Yield, 0.760 g, 83%. m.p. 573 K. Analysis, calculated for C₁₆H₁₂Cl₄CuN₂O₅: C 46.73, H 2.94, N 6.81; found: C 46.95, H 2.56, N 7.07%. The elemental analyses were performed with a Perkin Elmer PE2400II instrument.

S3. Refinement

C-bound H atoms were geometrically positioned (C—H 0.93–0.97 Å) and refined as riding, with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$. The water H atoms were located on a Fourier map and isotropically refined with the distance restraints O—H=0.85 (2) Å.

**Figure 1**

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted.

Aquabis(dichloroacetato- κ O)(1,10-phenanthroline- κ^2N,N')copper(II)

Crystal data

[Cu(C₂HCl₂O₂)₂(C₁₂H₈N₂)(H₂O)]

$M_r = 517.62$

Triclinic, $P\bar{1}$

$a = 8.2701$ (8) Å

$b = 10.8883$ (11) Å

$c = 12.0125$ (12) Å

$\alpha = 67.439$ (1)°

$\beta = 77.585$ (2)°

$\gamma = 73.776$ (2)°

$V = 952.02$ (16) Å³

$Z = 2$

$F(000) = 518$

$D_x = 1.806$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1923 reflections

$\theta = 2.3\text{--}27.1^\circ$

$\mu = 1.74$ mm⁻¹

$T = 273$ K

Block, colorless

$0.32 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.606$, $T_{\max} = 0.711$

5043 measured reflections

3346 independent reflections

2539 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.064$

$\theta_{\max} = 25.1^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -9 \rightarrow 8$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3346 reflections	$(\Delta/\sigma)_{\max} < 0.001$
261 parameters	$\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$
3 restraints	$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.23680 (6)	0.74569 (4)	0.41387 (4)	0.03375 (16)
Cl4	0.12884 (15)	0.83880 (10)	0.01776 (9)	0.0498 (3)
Cl3	0.18005 (19)	0.55281 (11)	0.05837 (10)	0.0653 (4)
Cl1	0.66991 (17)	0.90846 (12)	0.08639 (11)	0.0717 (4)
Cl2	0.5908 (2)	0.69108 (14)	0.04161 (11)	0.0831 (5)
O3	0.1567 (3)	0.7463 (2)	0.2733 (2)	0.0399 (6)
C5	0.2814 (4)	0.9060 (3)	0.5379 (3)	0.0310 (8)
O5	0.1749 (4)	0.5698 (3)	0.5130 (2)	0.0471 (7)
N2	0.1747 (4)	0.9522 (3)	0.3541 (2)	0.0324 (7)
N1	0.3082 (4)	0.7741 (3)	0.5489 (3)	0.0343 (7)
C9	0.0716 (5)	1.1808 (4)	0.2276 (3)	0.0447 (10)
H9	0.0263	1.2392	0.1564	0.054*
O2	0.7530 (4)	0.6097 (3)	0.2708 (2)	0.0586 (8)
Cl3	0.6067 (5)	0.6806 (4)	0.2683 (3)	0.0344 (8)
Cl6	0.0957 (5)	0.6794 (3)	0.1249 (3)	0.0340 (8)
H16	-0.0272	0.6861	0.1432	0.041*
Cl1	0.2127 (6)	1.1856 (4)	0.4993 (4)	0.0471 (10)
H11	0.1873	1.2779	0.4887	0.056*
Cl5	0.1639 (5)	0.6447 (3)	0.2447 (3)	0.0341 (8)
O4	0.2088 (4)	0.5243 (3)	0.3049 (2)	0.0609 (9)
Cl4	0.5542 (5)	0.7783 (4)	0.1437 (3)	0.0357 (9)
H14	0.4330	0.8198	0.1536	0.043*
Cl1	0.3872 (5)	0.6806 (4)	0.6436 (3)	0.0447 (10)
H1	0.4132	0.5893	0.6509	0.054*

C12	0.2859 (6)	1.0935 (4)	0.5985 (4)	0.0510 (11)
H12	0.3130	1.1242	0.6531	0.061*
C8	0.1025 (5)	1.2327 (4)	0.3051 (3)	0.0421 (10)
H8	0.0766	1.3264	0.2879	0.051*
C10	0.1075 (5)	1.0398 (4)	0.2542 (3)	0.0398 (9)
H10	0.0836	1.0063	0.2004	0.048*
C6	0.2062 (5)	1.0040 (3)	0.4314 (3)	0.0306 (8)
C7	0.1742 (5)	1.1436 (4)	0.4118 (3)	0.0368 (9)
C4	0.3223 (5)	0.9501 (4)	0.6208 (3)	0.0390 (9)
C2	0.4306 (6)	0.7160 (4)	0.7297 (4)	0.0506 (11)
H2	0.4810	0.6482	0.7955	0.061*
O1	0.5012 (4)	0.6801 (3)	0.3559 (2)	0.0634 (9)
C3	0.4009 (6)	0.8478 (4)	0.7199 (3)	0.0477 (10)
H3	0.4321	0.8710	0.7779	0.057*
H5A	0.192 (6)	0.535 (3)	0.458 (2)	0.065 (16)*
H5B	0.194 (6)	0.509 (3)	0.5816 (15)	0.068 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0471 (3)	0.0207 (2)	0.0318 (3)	-0.00140 (19)	-0.0107 (2)	-0.00826 (19)
C14	0.0728 (8)	0.0307 (5)	0.0416 (6)	-0.0135 (5)	-0.0179 (5)	-0.0005 (4)
C13	0.1158 (11)	0.0350 (6)	0.0486 (6)	-0.0027 (6)	-0.0209 (6)	-0.0222 (5)
C11	0.0801 (9)	0.0472 (7)	0.0746 (8)	-0.0293 (6)	-0.0338 (7)	0.0168 (6)
C12	0.1151 (12)	0.0745 (9)	0.0677 (8)	0.0119 (8)	-0.0340 (8)	-0.0440 (7)
O3	0.0622 (18)	0.0227 (13)	0.0366 (14)	-0.0029 (12)	-0.0151 (13)	-0.0119 (11)
C5	0.034 (2)	0.0258 (19)	0.0303 (18)	-0.0034 (15)	-0.0046 (16)	-0.0087 (15)
O5	0.073 (2)	0.0312 (15)	0.0346 (16)	-0.0132 (15)	-0.0142 (15)	-0.0038 (14)
N2	0.0419 (19)	0.0222 (16)	0.0315 (16)	-0.0044 (13)	-0.0051 (14)	-0.0090 (13)
N1	0.0420 (18)	0.0271 (17)	0.0326 (16)	-0.0042 (14)	-0.0059 (14)	-0.0104 (13)
C9	0.058 (3)	0.026 (2)	0.039 (2)	-0.0008 (18)	-0.014 (2)	-0.0011 (17)
O2	0.0396 (17)	0.0558 (19)	0.0453 (16)	0.0073 (15)	-0.0018 (14)	0.0063 (14)
C13	0.037 (2)	0.029 (2)	0.037 (2)	-0.0090 (17)	-0.0027 (18)	-0.0108 (17)
C16	0.041 (2)	0.0239 (19)	0.0350 (19)	-0.0038 (16)	-0.0062 (17)	-0.0094 (16)
C11	0.066 (3)	0.029 (2)	0.052 (2)	-0.010 (2)	-0.010 (2)	-0.018 (2)
C15	0.041 (2)	0.024 (2)	0.034 (2)	-0.0025 (16)	-0.0069 (17)	-0.0084 (16)
O4	0.113 (3)	0.0235 (15)	0.0449 (16)	0.0005 (16)	-0.0331 (17)	-0.0086 (13)
C14	0.032 (2)	0.030 (2)	0.039 (2)	-0.0029 (16)	-0.0048 (17)	-0.0088 (16)
C1	0.060 (3)	0.024 (2)	0.044 (2)	-0.0006 (19)	-0.018 (2)	-0.0048 (17)
C12	0.072 (3)	0.043 (3)	0.051 (3)	-0.018 (2)	-0.008 (2)	-0.026 (2)
C8	0.051 (3)	0.0200 (19)	0.047 (2)	-0.0035 (17)	-0.007 (2)	-0.0049 (17)
C10	0.051 (2)	0.030 (2)	0.035 (2)	-0.0034 (18)	-0.0145 (18)	-0.0065 (17)
C6	0.034 (2)	0.0242 (19)	0.0298 (18)	-0.0039 (15)	0.0009 (15)	-0.0097 (15)
C7	0.040 (2)	0.0229 (19)	0.042 (2)	-0.0055 (16)	-0.0010 (18)	-0.0088 (17)
C4	0.044 (2)	0.039 (2)	0.036 (2)	-0.0094 (18)	-0.0024 (18)	-0.0149 (18)
C2	0.063 (3)	0.043 (3)	0.040 (2)	-0.005 (2)	-0.020 (2)	-0.006 (2)
O1	0.0491 (19)	0.083 (2)	0.0386 (16)	0.0057 (16)	-0.0020 (15)	-0.0158 (16)
C3	0.057 (3)	0.052 (3)	0.038 (2)	-0.010 (2)	-0.014 (2)	-0.016 (2)

Geometric parameters (Å, °)

Cu1—O3	1.939 (2)	C13—O1	1.213 (4)
Cu1—O5	1.971 (2)	C13—C14	1.536 (5)
Cu1—N1	1.994 (3)	C16—C15	1.531 (5)
Cu1—N2	2.027 (3)	C16—H16	0.9800
Cu1—O1	2.152 (3)	C11—C12	1.359 (6)
C14—C16	1.774 (3)	C11—C7	1.417 (5)
C13—C16	1.759 (4)	C11—H11	0.9300
C11—C14	1.767 (4)	C15—O4	1.223 (4)
C12—C14	1.753 (4)	C14—H14	0.9800
O3—C15	1.261 (4)	C1—C2	1.374 (5)
C5—N1	1.348 (4)	C1—H1	0.9300
C5—C4	1.394 (5)	C12—C4	1.432 (5)
C5—C6	1.444 (5)	C12—H12	0.9300
O5—H5A	0.85 (3)	C8—C7	1.410 (5)
O5—H5B	0.85 (3)	C8—H8	0.9300
N2—C10	1.331 (4)	C10—H10	0.9300
N2—C6	1.355 (4)	C6—C7	1.401 (5)
N1—C1	1.348 (4)	C4—C3	1.411 (5)
C9—C8	1.355 (5)	C2—C3	1.349 (5)
C9—C10	1.399 (5)	C2—H2	0.9300
C9—H9	0.9300	C3—H3	0.9300
O2—C13	1.240 (5)		
C11...C14 ⁱ	3.306 (2)	Cg1...Cg2 ⁱⁱⁱ	3.734 (2)
C12...C13 ⁱⁱ	3.278 (2)		
O3—Cu1—O5	91.06 (10)	O4—C15—O3	127.3 (3)
O3—Cu1—N1	171.76 (11)	O4—C15—C16	117.8 (3)
O5—Cu1—N1	95.86 (11)	O3—C15—C16	114.7 (3)
O3—Cu1—N2	90.28 (11)	C13—C14—C12	110.9 (3)
O5—Cu1—N2	149.53 (12)	C13—C14—C11	109.3 (2)
N1—Cu1—N2	81.49 (11)	C12—C14—C11	110.0 (2)
O3—Cu1—O1	95.15 (11)	C13—C14—H14	108.9
O5—Cu1—O1	101.24 (12)	C12—C14—H14	108.9
N1—Cu1—O1	87.88 (12)	C11—C14—H14	108.9
N2—Cu1—O1	108.94 (12)	N1—C1—C2	122.1 (4)
C15—O3—Cu1	127.3 (2)	N1—C1—H1	118.9
N1—C5—C4	124.2 (3)	C2—C1—H1	119.0
N1—C5—C6	115.7 (3)	C11—C12—C4	121.4 (4)
C4—C5—C6	120.1 (3)	C11—C12—H12	119.3
Cu1—O5—H5A	99 (2)	C4—C12—H12	119.3
Cu1—O5—H5B	137 (3)	C9—C8—C7	119.6 (3)
H5A—O5—H5B	111 (3)	C9—C8—H8	120.2
C10—N2—C6	117.7 (3)	C7—C8—H8	120.2
C10—N2—Cu1	129.8 (3)	N2—C10—C9	121.9 (4)
C6—N2—Cu1	112.5 (2)	N2—C10—H10	119.0

C1—N1—C5	117.1 (3)	C9—C10—H10	119.1
C1—N1—Cu1	128.6 (3)	N2—C6—C7	124.1 (3)
C5—N1—Cu1	114.1 (2)	N2—C6—C5	116.1 (3)
C8—C9—C10	120.4 (4)	C7—C6—C5	119.8 (3)
C8—C9—H9	119.8	C6—C7—C8	116.3 (3)
C10—C9—H9	119.8	C6—C7—C11	118.9 (3)
O1—C13—O2	125.7 (4)	C8—C7—C11	124.7 (3)
O1—C13—C14	117.0 (3)	C5—C4—C3	116.3 (3)
O2—C13—C14	117.3 (3)	C5—C4—C12	118.5 (3)
C15—C16—C13	113.0 (3)	C3—C4—C12	125.2 (3)
C15—C16—C14	112.4 (2)	C3—C2—C1	120.8 (3)
C13—C16—C14	109.30 (19)	C3—C2—H2	119.6
C15—C16—H16	107.3	C1—C2—H2	119.6
C13—C16—H16	107.3	C13—O1—Cu1	144.6 (3)
C14—C16—H16	107.3	C2—C3—C4	119.4 (3)
C12—C11—C7	121.2 (4)	C2—C3—H3	120.3
C12—C11—H11	119.4	C4—C3—H3	120.3
C7—C11—H11	119.4		

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

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C16—H16 \cdots O2 ^{iv}	0.98	2.24	3.118 (5)	149
O5—H5B \cdots O2 ^v	0.85 (2)	1.81 (2)	2.654 (3)	174 (3)
O5—H5A \cdots O4	0.85 (2)	1.86 (2)	2.673 (4)	159 (3)

Symmetry codes: (iv) $x-1, y, z$; (v) $-x+1, -y+1, -z+1$.