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Chlorido{μ-2,6-bis[(2-aminoethyl)iminomethyl]-4-chlorophenolato}-μ-oxido-dicopper(II) trihydrate

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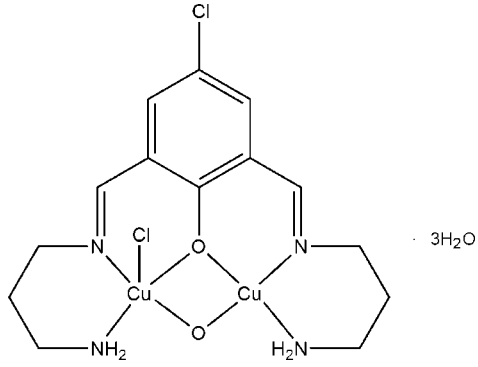
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.010 Å; R factor = 0.061; wR factor = 0.175; data-to-parameter ratio = 16.8.

In the title dinuclear complex, $[Cu_2(C_{14}H_{20}ClN_4O)ClO]\cdot 3H_2O$, one Cu^{II} cation assumes a distorted square-planar coordination geometry and the other a distorted square-pyramidal coordination geometry. Both Cu^{II} cations are N,N',O-chelated by one arm of the 2,6-bis[(2-aminoethyl)iminomethyl]-4-chlorophenolate anion, and one oxide anion bridges the two Cu^{II} cations, forming a dinuclear complex. One of the Cu^{II} cations is further coordinated by an Cl^- anion in the apical direction. In the crystal, lattice water molecules are linked with the complex molecule *via* O—H···Cl hydrogen bonds while O—H···O hydrogen bonding occurs between lattice water molecules , forming three-dimensional network structure.

Related literature

For the synthesis, see: Gagne *et al.* (1981). For a related oxygen anion-bridging complex, see: Olmstead *et al.* (2011). For the biological activity of Schiff bases, see: Raman *et al.* (2007); Hao *et al.* (2006). For the biological properties of binuclear complexes, see: Tian *et al.* (2007); Anbu *et al.* (2009). Several proteins *in vivo* contain transition metal atoms, especially, Cu^{II}, see: Dede *et al.* (2009); Veysel *et al.* (2003); Asokan *et al.* (1995).



Experimental

Crystal data

$[Cu_2(C_{14}H_{20}ClN_4O)ClO]\cdot 3H_2O$
M_r = 528.37
Monoclinic, $P2_1/c$
a = 11.201 (5) Å
b = 12.387 (7) Å
c = 16.718 (7) Å
β = 93.18 (4)°
V = 2316.0 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.10 mm^{-1}
T = 291 K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.572, T_{max} = 0.633
12029 measured reflections
4087 independent reflections
3286 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.175
S = 1.02
4087 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WD···Cl1	0.85	1.90	2.583 (12)	136
O2W—H2WB···O3W	0.85	2.57	3.114 (13)	123
O3W—H3WD···Cl2	0.85	2.70	3.478 (10)	152

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5529).

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Chlorido{μ-2,6-bis[(2-aminoethyl)iminomethyl]-4-chlorophenolato}-μ-oxido-dicopper(II) trihydrate

Jing-Jing Zhou, Wei Xiao, Jia-Wei Mao and Hong Zhou

S1. Comment

Schiff bases have received special attention of biochemists because of their biological activities (Raman *et al.*, 2007; Hao *et al.*, 2006). Researches show that binuclear complexes have good biological properties (Tian *et al.*, 2007; Anbu *et al.*, 2009). Several proteins in vivo contain transition metal centers, especially, the Cu(II) centers (Dede *et al.*, 2009; Veysel *et al.*, 2003). Thus, in this paper, we report on the synthesis and the crystal structure of a new binuclear copper complex. Although a similar complex has been reported in the literature (Asokan *et al.*, 1995), however, the title complex has different substituent in the phenoxid group and counter anion with the reported complex. The crystal structure of the title complex is shown in Fig.1. The molecular unit contains a chloride anion and two copper ions. The coordination environment of the two copper ions are different. Cu2 has four coordinated atoms with quadrilateral configuration, all the atoms locate in an approximately plane with a mean plane derivation of 0.072 Å. While Cu1 has five coordinated atoms with a square pyramid configuration and the chloride anion occupies the apical position with Cu1-Cl2 distance of 2.484 Å. The basal plane is composed of two imino nitrogen atoms, one phenoxide atom and one oxygen anion derived from the solvent of H2O with a mean plane derivation of 0.016 Å. This oxygen anion bridged structure is also found in a dinuclear complex which was obtained by a similar experimental condition (Olmstead *et al.*, 2011).

S2. Experimental

2,6-Diformyl-4-chlorophenol was prepared according to the literature methods (Gagne *et al.*, 1981). 2,6-Diformyl-4-chlorophenol (0.25 mmol, 0.046 g) in absolute methanol (10 ml) was added to a methanol solution (10 ml) containing 1,3-propanediamine (0.5 mmol, 0.037 g). The solution was stirred vigorously for 2 h at room temperature. Afterwards, a methanol solution (10 ml) of $CuCl_2.2H_2O$ (0.5 mmol, 0.085 g) was added dropwise, the mixture was stirred for a further 6 h at ambient temperature. The dark-green block-shaped crystals suitable for X-ray structure analysis were obtained by evaporating the methanol solution of the complex over a period of one month.

S3. Refinement

H atoms were placed in calculated positions with 0.93–0.97 Å and O—H = 0.85 Å, and included in the refinement in the riding-model approximation, with U(H)=1.2–1.5U_{eq}(C,O).

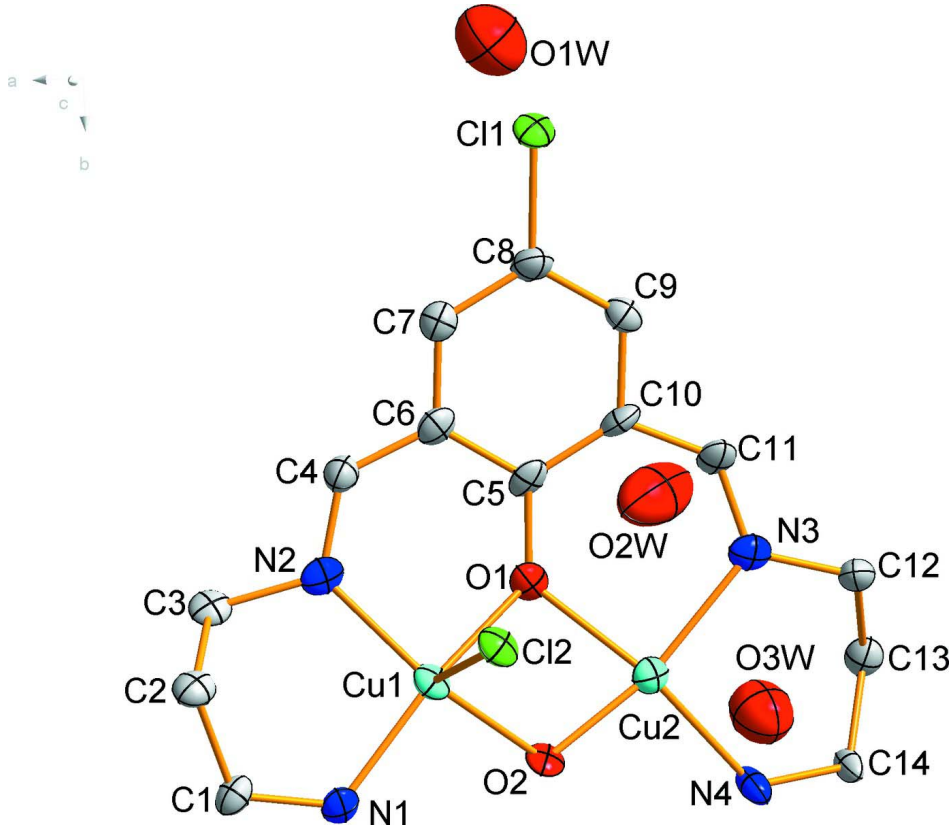

Figure 1

A view of (I), showing the labeling of the non-H atoms and 30% probability ellipsoids. H atoms have been omitted for clarity.

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$Z = 4$
$F(000) = 1080$
$D_x = 1.515$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4001 reflections
$\theta = 2.4$–26.6°
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Block, green
0.30 × 0.26 × 0.24 mm

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Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
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$T_{min} = 0.572$, $T_{max} = 0.633$
12029 measured reflections
4087 independent reflections
3286 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -13\rightarrow13$
$k = -14\rightarrow11$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.175$
$S = 1.02$
4087 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 12.660P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.076$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
Cl1	0.29197 (15)	0.09726 (13)	0.30847 (10)	0.0409 (4)
Cl2	0.31005 (15)	0.62287 (14)	0.44102 (10)	0.0435 (4)
Cu1	0.43928 (7)	0.66390 (6)	0.32886 (5)	0.0360 (2)
Cu2	0.22384 (7)	0.67193 (6)	0.21370 (5)	0.0360 (2)
C1	0.6375 (6)	0.7673 (6)	0.4411 (4)	0.0388 (15)
H1A	0.6233	0.8117	0.4874	0.047*
H1B	0.7089	0.7953	0.4180	0.047*
C2	0.6665 (7)	0.6538 (6)	0.4715 (4)	0.0451 (17)
H2A	0.6055	0.6302	0.5066	0.054*
H2B	0.7427	0.6541	0.5020	0.054*
C3	0.6721 (6)	0.5750 (5)	0.4003 (4)	0.0376 (15)
H3A	0.7219	0.6064	0.3607	0.045*
H3B	0.7101	0.5086	0.4191	0.045*
C4	0.5264 (6)	0.4435 (6)	0.3522 (4)	0.0395 (15)
H4	0.5824	0.3950	0.3744	0.047*
C5	0.3361 (6)	0.4596 (5)	0.2694 (4)	0.0360 (15)
C6	0.4249 (6)	0.3996 (6)	0.3141 (4)	0.0412 (16)
C7	0.4106 (6)	0.2905 (6)	0.3267 (4)	0.0358 (14)
H7	0.4677	0.2524	0.3577	0.043*
C8	0.3091 (7)	0.2369 (6)	0.2923 (4)	0.0460 (17)
C9	0.2214 (6)	0.2954 (5)	0.2455 (4)	0.0369 (14)
H9	0.1554	0.2602	0.2215	0.044*
C10	0.2354 (6)	0.4051 (5)	0.2363 (4)	0.0396 (15)
C11	0.1424 (6)	0.4496 (5)	0.1867 (4)	0.0409 (16)
H11	0.0913	0.3989	0.1621	0.049*

C12	0.0115 (6)	0.5819 (6)	0.1123 (5)	0.0472 (18)
H12A	−0.0533	0.6059	0.1440	0.057*
H12B	−0.0157	0.5176	0.0837	0.057*
C13	0.0339 (7)	0.6702 (6)	0.0498 (4)	0.0428 (16)
H13A	−0.0303	0.6710	0.0084	0.051*
H13B	0.1087	0.6570	0.0249	0.051*
C14	0.0392 (6)	0.7802 (5)	0.0960 (4)	0.0376 (15)
H14A	0.0569	0.8361	0.0578	0.045*
H14B	−0.0403	0.7947	0.1136	0.045*
N1	0.5352 (5)	0.7852 (5)	0.3811 (3)	0.0398 (13)
H1C	0.5640	0.8243	0.3411	0.048*
H1D	0.4827	0.8279	0.4050	0.048*
N2	0.5521 (5)	0.5481 (5)	0.3605 (3)	0.0417 (13)
N3	0.1152 (5)	0.5507 (5)	0.1690 (3)	0.0405 (13)
N4	0.1253 (5)	0.7929 (5)	0.1670 (3)	0.0437 (14)
H4A	0.0830	0.8191	0.2069	0.052*
H4B	0.1768	0.8452	0.1545	0.052*
O1	0.3458 (4)	0.5674 (4)	0.2586 (2)	0.0373 (10)
O2	0.3320 (4)	0.7525 (3)	0.2702 (3)	0.0360 (10)
O1W	0.2820 (9)	−0.0067 (9)	0.4419 (7)	0.144 (4)
H1WD	0.2653	0.0494	0.4142	0.173*
H1WC	0.2692	0.0055	0.4907	0.216*
O2W	0.1297 (9)	0.4729 (8)	0.3981 (7)	0.150 (4)
H2WD	0.1802	0.4946	0.3656	0.180*
H2WB	0.1094	0.5253	0.4272	0.224*
O3W	0.0267 (9)	0.7040 (8)	0.3693 (5)	0.120 (3)
H3WD	0.0988	0.6829	0.3681	0.144*
H3WA	−0.0136	0.6575	0.3937	0.181*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0444 (9)	0.0364 (9)	0.0429 (9)	−0.0072 (7)	0.0111 (7)	0.0118 (7)
Cl2	0.0412 (9)	0.0478 (10)	0.0426 (9)	−0.0115 (7)	0.0131 (7)	0.0021 (7)
Cu1	0.0350 (4)	0.0388 (5)	0.0352 (4)	−0.0085 (3)	0.0097 (3)	0.0019 (3)
Cu2	0.0359 (4)	0.0376 (5)	0.0352 (4)	0.0013 (3)	0.0082 (3)	0.0003 (3)
C1	0.038 (3)	0.045 (4)	0.034 (3)	0.009 (3)	0.007 (3)	0.010 (3)
C2	0.047 (4)	0.039 (4)	0.050 (4)	−0.003 (3)	0.014 (3)	0.014 (3)
C3	0.046 (4)	0.036 (3)	0.033 (3)	−0.005 (3)	0.015 (3)	0.016 (3)
C4	0.034 (3)	0.040 (4)	0.044 (4)	0.003 (3)	0.003 (3)	0.005 (3)
C5	0.040 (3)	0.039 (4)	0.030 (3)	0.017 (3)	0.009 (3)	−0.010 (3)
C6	0.038 (4)	0.042 (4)	0.044 (4)	0.012 (3)	0.012 (3)	−0.006 (3)
C7	0.038 (3)	0.043 (4)	0.026 (3)	0.002 (3)	0.006 (3)	0.003 (3)
C8	0.054 (4)	0.032 (4)	0.051 (4)	0.007 (3)	0.000 (3)	−0.008 (3)
C9	0.039 (4)	0.038 (3)	0.035 (3)	−0.007 (3)	0.006 (3)	−0.001 (3)
C10	0.047 (4)	0.028 (3)	0.044 (4)	0.016 (3)	0.000 (3)	0.007 (3)
C11	0.047 (4)	0.035 (4)	0.041 (4)	0.011 (3)	−0.002 (3)	−0.016 (3)
C12	0.038 (4)	0.031 (4)	0.073 (5)	0.002 (3)	−0.003 (3)	−0.008 (3)

C13	0.043 (4)	0.047 (4)	0.038 (4)	0.005 (3)	0.001 (3)	−0.005 (3)
C14	0.038 (3)	0.032 (3)	0.040 (4)	−0.011 (3)	−0.020 (3)	0.017 (3)
N1	0.036 (3)	0.040 (3)	0.044 (3)	0.009 (2)	0.008 (2)	−0.015 (3)
N2	0.047 (3)	0.042 (3)	0.037 (3)	0.007 (3)	0.016 (3)	−0.002 (2)
N3	0.046 (3)	0.039 (3)	0.038 (3)	0.002 (3)	0.014 (2)	−0.007 (2)
N4	0.044 (3)	0.045 (3)	0.040 (3)	−0.020 (3)	−0.014 (3)	0.010 (3)
O1	0.036 (2)	0.043 (3)	0.034 (2)	0.001 (2)	0.0127 (19)	−0.0118 (19)
O2	0.036 (2)	0.032 (2)	0.041 (2)	−0.0120 (19)	0.0114 (19)	0.0163 (19)
O1W	0.139 (9)	0.154 (9)	0.141 (9)	−0.022 (7)	0.014 (7)	−0.009 (7)
O2W	0.133 (8)	0.115 (8)	0.208 (12)	0.016 (6)	0.076 (8)	0.047 (8)
O3W	0.123 (7)	0.119 (7)	0.118 (7)	−0.016 (6)	0.000 (6)	0.015 (6)

Geometric parameters (Å, º)

Cl1—C8	1.763 (7)	C7—C8	1.411 (10)
Cl2—Cu1	2.484 (2)	C7—H7	0.9300
Cu1—O2	1.865 (4)	C8—C9	1.420 (10)
Cu1—O1	1.941 (4)	C9—C10	1.377 (9)
Cu1—N2	1.965 (6)	C9—H9	0.9300
Cu1—N1	2.017 (6)	C10—C11	1.408 (9)
Cu1—Cu2	3.0040 (18)	C11—N3	1.319 (9)
Cu2—O2	1.797 (4)	C11—H11	0.9300
Cu2—N4	1.994 (6)	C12—N3	1.508 (9)
Cu2—O1	1.997 (5)	C12—C13	1.542 (10)
Cu2—N3	2.048 (6)	C12—H12A	0.9700
C1—N1	1.498 (8)	C12—H12B	0.9700
C1—C2	1.524 (9)	C13—C14	1.565 (9)
C1—H1A	0.9700	C13—H13A	0.9700
C1—H1B	0.9700	C13—H13B	0.9700
C2—C3	1.543 (10)	C14—N4	1.496 (7)
C2—H2A	0.9700	C14—H14A	0.9700
C2—H2B	0.9700	C14—H14B	0.9700
C3—N2	1.503 (9)	N1—H1C	0.9000
C3—H3A	0.9700	N1—H1D	0.9000
C3—H3B	0.9700	N4—H4A	0.9000
C4—N2	1.333 (9)	N4—H4B	0.9000
C4—C6	1.384 (10)	O1W—H1WD	0.8501
C4—H4	0.9300	O1W—H1WC	0.8499
C5—O1	1.353 (8)	O2W—H2WD	0.8496
C5—C10	1.401 (10)	O2W—H2WB	0.8500
C5—C6	1.420 (9)	O3W—H3WD	0.8500
C6—C7	1.378 (10)	O3W—H3WA	0.8501
O2—Cu1—O1	74.6 (2)	C7—C8—C9	120.1 (6)
O2—Cu1—N2	163.2 (2)	C7—C8—Cl1	119.4 (5)
O1—Cu1—N2	91.8 (2)	C9—C8—Cl1	120.5 (5)
O2—Cu1—N1	95.8 (2)	C10—C9—C8	119.0 (6)
O1—Cu1—N1	167.6 (2)	C10—C9—H9	120.5

N2—Cu1—N1	96.2 (2)	C8—C9—H9	120.5
O2—Cu1—Cl2	97.57 (13)	C9—C10—C5	121.7 (6)
O1—Cu1—Cl2	90.79 (13)	C9—C10—C11	111.5 (6)
N2—Cu1—Cl2	92.30 (16)	C5—C10—C11	126.7 (6)
N1—Cu1—Cl2	98.30 (17)	N3—C11—C10	131.2 (7)
O2—Cu1—Cu2	34.16 (13)	N3—C11—H11	114.4
O1—Cu1—Cu2	41.00 (14)	C10—C11—H11	114.4
N2—Cu1—Cu2	132.74 (18)	N3—C12—C13	117.3 (6)
N1—Cu1—Cu2	129.95 (17)	N3—C12—H12A	108.0
Cl2—Cu1—Cu2	90.55 (6)	C13—C12—H12A	108.0
O2—Cu2—N4	97.5 (2)	N3—C12—H12B	108.0
O2—Cu2—O1	74.66 (19)	C13—C12—H12B	108.0
N4—Cu2—O1	170.4 (2)	H12A—C12—H12B	107.2
O2—Cu2—N3	165.6 (2)	C12—C13—C14	106.7 (5)
N4—Cu2—N3	95.9 (2)	C12—C13—H13A	110.4
O1—Cu2—N3	92.4 (2)	C14—C13—H13A	110.4
O2—Cu2—Cu1	35.64 (14)	C12—C13—H13B	110.4
N4—Cu2—Cu1	133.09 (16)	C14—C13—H13B	110.4
O1—Cu2—Cu1	39.61 (13)	H13A—C13—H13B	108.6
N3—Cu2—Cu1	130.51 (17)	N4—C14—C13	119.2 (5)
N1—C1—C2	120.0 (6)	N4—C14—H14A	107.5
N1—C1—H1A	107.3	C13—C14—H14A	107.5
C2—C1—H1A	107.3	N4—C14—H14B	107.5
N1—C1—H1B	107.3	C13—C14—H14B	107.5
C2—C1—H1B	107.3	H14A—C14—H14B	107.0
H1A—C1—H1B	106.9	C1—N1—Cu1	123.3 (4)
C1—C2—C3	110.1 (6)	C1—N1—H1C	106.5
C1—C2—H2A	109.6	Cu1—N1—H1C	106.5
C3—C2—H2A	109.6	C1—N1—H1D	106.5
C1—C2—H2B	109.6	Cu1—N1—H1D	106.5
C3—C2—H2B	109.6	H1C—N1—H1D	106.5
H2A—C2—H2B	108.2	C4—N2—C3	116.4 (6)
N2—C3—C2	114.1 (5)	C4—N2—Cu1	123.3 (5)
N2—C3—H3A	108.7	C3—N2—Cu1	120.2 (4)
C2—C3—H3A	108.7	C11—N3—C12	123.0 (6)
N2—C3—H3B	108.7	C11—N3—Cu2	119.3 (5)
C2—C3—H3B	108.7	C12—N3—Cu2	117.5 (4)
H3A—C3—H3B	107.6	C14—N4—Cu2	123.4 (4)
N2—C4—C6	126.7 (6)	C14—N4—H4A	106.5
N2—C4—H4	116.7	Cu2—N4—H4A	106.5
C6—C4—H4	116.7	C14—N4—H4B	106.5
O1—C5—C10	119.5 (6)	Cu2—N4—H4B	106.5
O1—C5—C6	121.8 (6)	H4A—N4—H4B	106.5
C10—C5—C6	118.7 (6)	C5—O1—Cu1	124.8 (4)
C7—C6—C4	114.4 (6)	C5—O1—Cu2	129.2 (4)
C7—C6—C5	120.6 (7)	Cu1—O1—Cu2	99.4 (2)
C4—C6—C5	124.8 (7)	Cu2—O2—Cu1	110.2 (2)
C6—C7—C8	119.8 (6)	H1WD—O1W—H1WC	109.5

C6—C7—H7	120.1	H2WD—O2W—H2WB	109.5
C8—C7—H7	120.1	H3WD—O3W—H3WA	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WD*···Cl1	0.85	1.90	2.583 (12)	136
O2*W*—H2*WB*···O3*W*	0.85	2.57	3.114 (13)	123
O3*W*—H3*WD*···Cl2	0.85	2.70	3.478 (10)	152