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[(2*S*)-2-(3,5-Dichloro-2-oxidobenzylideneamino)-3-(4-hydroxyphenyl)propionato- κ^3 O,N,O'](dimethylformamide- κ O)copper(II)

 Ming-Xiong Tan,^{a,b*} Zhen-Feng Chen,^c Zhou Neng^b and Hong Liang^a

^aCollege of Chemistry and Chemical Engineering, Central South University, Changsha, Hunan 410083, People's Republic of China, ^bDepartment of Chemistry and Biology, Yu Lin Normal College, Yulin, Guangxi 537000, People's Republic of China, and ^cKey Laboratory of Medicinal Chemical Resources and Molecular Engineering, Ministry of Education, College of Chemistry and Chemical Engineering, Guangxi Normal University, Yucui Road 15, Guilin 541004, People's Republic of China

Correspondence e-mail: tanmx00@163.com

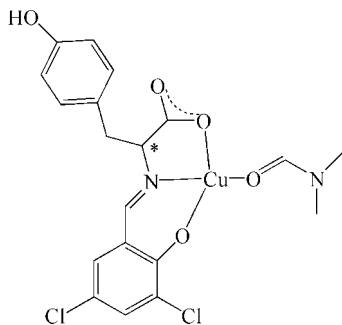
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.061; wR factor = 0.148; data-to-parameter ratio = 13.9.

In the title complex, $[\text{Cu}(\text{C}_{16}\text{H}_{11}\text{Cl}_2\text{NO}_4)(\text{C}_3\text{H}_7\text{NO})]$, the Cu^{II} atom is coordinated by two O atoms and one N atom from the tridentate ligand L^{2-} { $\text{LH}_2 = (2S)$ -[2-(3,5-dichloro-2-hydroxybenzylidene)imino]-3-(4-hydroxyphenyl)propionic acid} and one O atom from a dimethylformamide molecule, resulting in a slightly distorted square-planar geometry. The structure forms a one-dimensional chain through weak coordination bonds [Cu \cdots O 3.080 (1), Cu \cdots Cl 3.269 (1) Å] and a three-dimensional network through O—H \cdots O and C—H \cdots O hydrogen bonds.

Related literature

For related structures, see: Li *et al.* (2008); Zhang, Li *et al.* (2007); Zhang, Feng *et al.* (2007*a,b*). For related literature, see: Xia *et al.* (2007); Liu *et al.* (2007); Cohen *et al.* (1964); Desiraju (1989); Zordan *et al.* (2005).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{16}\text{H}_{11}\text{Cl}_2\text{NO}_4)(\text{C}_3\text{H}_7\text{NO})]$ $V = 2081.7$ (7) Å³
 $M_r = 488.79$ $Z = 4$
 Orthorhombic, $P2_12_12_1$ Mo $K\alpha$ radiation
 $a = 5.8646$ (16) Å $\mu = 1.34$ mm⁻¹
 $b = 13.220$ (2) Å $T = 298$ (2) K
 $c = 26.850$ (3) Å $0.48 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer 10650 measured reflections
 3638 independent reflections
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996) 2915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.098$
 $T_{\text{min}} = 0.532$, $T_{\text{max}} = 0.786$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$ $\Delta\rho_{\text{max}} = 0.50$ e Å⁻³
 $wR(F^2) = 0.148$ $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³
 $S = 1.04$ Absolute structure: Flack (1983),
 3638 reflections with 1505 Friedel pairs
 262 parameters Flack parameter: 0.04 (3)
 H-atom parameters constrained

Table 1

Selected geometric parameters (Å, °).

Cu1—O4	1.875 (5)	Cu1—N1	1.934 (5)
Cu1—O1	1.931 (5)	Cu1—O5	1.954 (4)
O4—Cu1—O1	169.0 (2)	O4—Cu1—O5	90.2 (2)
O4—Cu1—N1	94.2 (2)	O1—Cu1—O5	91.9 (2)
O1—Cu1—N1	84.5 (2)	N1—Cu1—O5	174.3 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots O2 ⁱ	0.82	1.87	2.661 (7)	163
C17—H17 \cdots O4	0.93	2.27	2.743 (8)	111
C18—H18B \cdots O1 ⁱⁱ	0.96	2.54	3.421 (10)	150

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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: RT2016).

References

- Bruker (2001). *SAINTE* and *SMART*. Bruker AXS Inc, Madison, Wisconsin, USA.
- Cohen, M. D., Schmidt, G. M. & Sonntag, F. I. (1964). *J. Chem. Soc.* pp. 2000–2013.
- Desiraju, G. R. (1989). *Crystal Engineering: The Design of Organic Solids*. Amsterdam: Elsevier.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Li, G. Z., Zhang, S. H. & Liu, Z. (2008). *Acta Cryst.* **E64**, m52.
- Liu, Z., Zhang, S.-H., Feng, X.-Z., Li, G.-Z. & Lin, Y.-B. (2007). *Acta Cryst.* **E63**, m156–m158.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Xia, J. H., Zhang, S.-H., Feng, X.-Z., Jin, L.-X. & Zheng, L. (2007). *Acta Cryst.* **E63**, m353–m355.
- Zhang, S.-H., Feng, X.-Z., Li, G.-Z., Jing, L.-X. & Liu, Z. (2007a). *Acta Cryst.* **E63**, m1156–m1157.
- Zhang, S.-H., Feng, X.-Z., Li, G.-Z., Jing, L.-X. & Liu, Z. (2007b). *Acta Cryst.* **E63**, m535–m536.
- Zhang, S.-H., Li, G.-Z., Feng, X.-Z. & Liu, Z. (2007). *Acta Cryst.* **E63**, m1319–m1320.
- Zordan, F., Brammer, L. & Sherwood, P. (2005). *J. Am. Chem. Soc.* **127**, 5979–5989.

supporting information

Acta Cryst. (2008). E64, m599–m600 [doi:10.1107/S1600536808007939]

[(2*S*)-2-(3,5-Dichloro-2-oxidobenzylideneamino)-3-(4-hydroxyphenyl)-propionato- κ^3 O,N,O'](dimethylformamide- κ O)copper(II)

Ming-Xiong Tan, Zhen-Feng Chen, Zhou Neng and Hong Liang

S1. Comment

Halogens have a ubiquitous presence in both inorganic and organic chemistry, serving as monodentate or bridging ligands for a wide variety of d-block, f-block, and main group metals as well being common substituents in a large number of organic compounds. Most frequently they lie at the periphery of molecules. The resultant steric accessibility has the potential for halogenated compounds to be attractive targets for use in supramolecular chemistry and crystal engineering wherein the halogen atoms are directly involved in intermolecular interactions. Indeed, interest in packing arrangements of halogenated compounds goes back many years to what Schmidt called the chloro effect, wherein the presence of chloro substituents on aromatic compounds frequently resulted in stacking arrangements with a resultant short (*ca* 4 Å) crystallographic axis. (Cohen *et al.*, 1964; Zordan *et al.*, 2005; Cohen *et al.*, 1964; Desiraju, 1989; Zhang, Li *et al.*, 2007). Herein, we chose LH_2 as ligand system, and obtained a new mononuclear copper complex [Cu(L)(C₃H₇NO)] (1).

The title compound, (I), is a chiral Cu^{II} complex containing a dimethylformamide and a chiral ligand constructed from 3,5-Dichloro-2-hydroxy-benzaldehyde and 2-Amino-3-(4-hydroxy-phenyl)-propionic acid. The asymmetric unit of (I) shows a complex consisting of one Cu^{II} atom, one L^2 ligand and one dimethylformamide (Fig. 1). The Cu atom is coordinated by two oxygen atoms and one N atom from one tridentate L^2 ligand, to yield a slightly distorted planar geometry with bond lengths Cu1—O1, Cu1—O4, Cu1—O5 and Cu1—N1 1.931 (5), 1.875 (5), 1.954 (4) and 1.934 (5) Å, respectively; and bond angles (*cis*-angles are in the range of 84.5 (2)–91.9 (2) °, but all *trans*-angles are 169.0 (2)–174.3 (2) °) (Table 2).

As expected, all other bond distances and angles are within normal range. The structure forms a one-dimensional chain (Fig. 2) through weak coordination bonds (Cu1—O2ⁱ, 3.080 (1) Å, Cu1—C11ⁱⁱ, 3.269 (1) Å, symmetry codes: i: 1 + x, y, z; ii: -1 + x, y, z) and a three-dimensional network *via* weak hydrogen bonds: (O3—H3ⁱⁱⁱ···O2ⁱ, 2.661 (7) Å, symmetry codes: i: 1 - x, 1/2 + y, 3/2 - z) and C—Hⁱⁱⁱⁱ···O hydrogen bond (C17—H17ⁱⁱⁱⁱ···O4, 2.743 (8) Å, C18—H18Bⁱⁱⁱⁱ···O1ⁱⁱ, 2.536 (4) Å, symmetry code: ii: 1/2 + x, -1/2 - y, 2 - z) (Fig. 3).

S2. Experimental

3,5-Dichloro-2-hydroxy-benzaldehyde (0.382 g, 2.0 mmol) and 2-Amino-3-(4-hydroxy-phenyl)-propionic acid (0.3624 g, 2.0 mmol) were dissolved in 10 ml absolute methanol. The mixture was stirred for 1 h at room temperature to yield a yellow solution. To this was added a solution of CuSO₄·5H₂O (0.5 g, 2 mmol) in a mixture of 2 ml DMF and 10 ml methanol. The mixture was refluxed for 1 h, and then the blue solution was filtered. Blue single crystals suitable for X-ray analysis were obtained by slow evaporation of the above filtrate at room temperature. Yield: 89.6% (based on Copper). Elemental analysis for [Cu(C₁₆H₁₁Cl₂NO₄)(C₃H₇NO)] calculated: C 46.69, H 3.71, N 5.73%; found: C 46.61, H 3.84, N 5.67%.

S3. Refinement

All hydrogen atoms were positioned geometrically and refined with a riding model, with distances 0.96 (CH₃) or 0.93 Å (aromatic rings), and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{aromatic ring})$ or $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{CH}_3)$, O—H distance: 0.82 Å with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

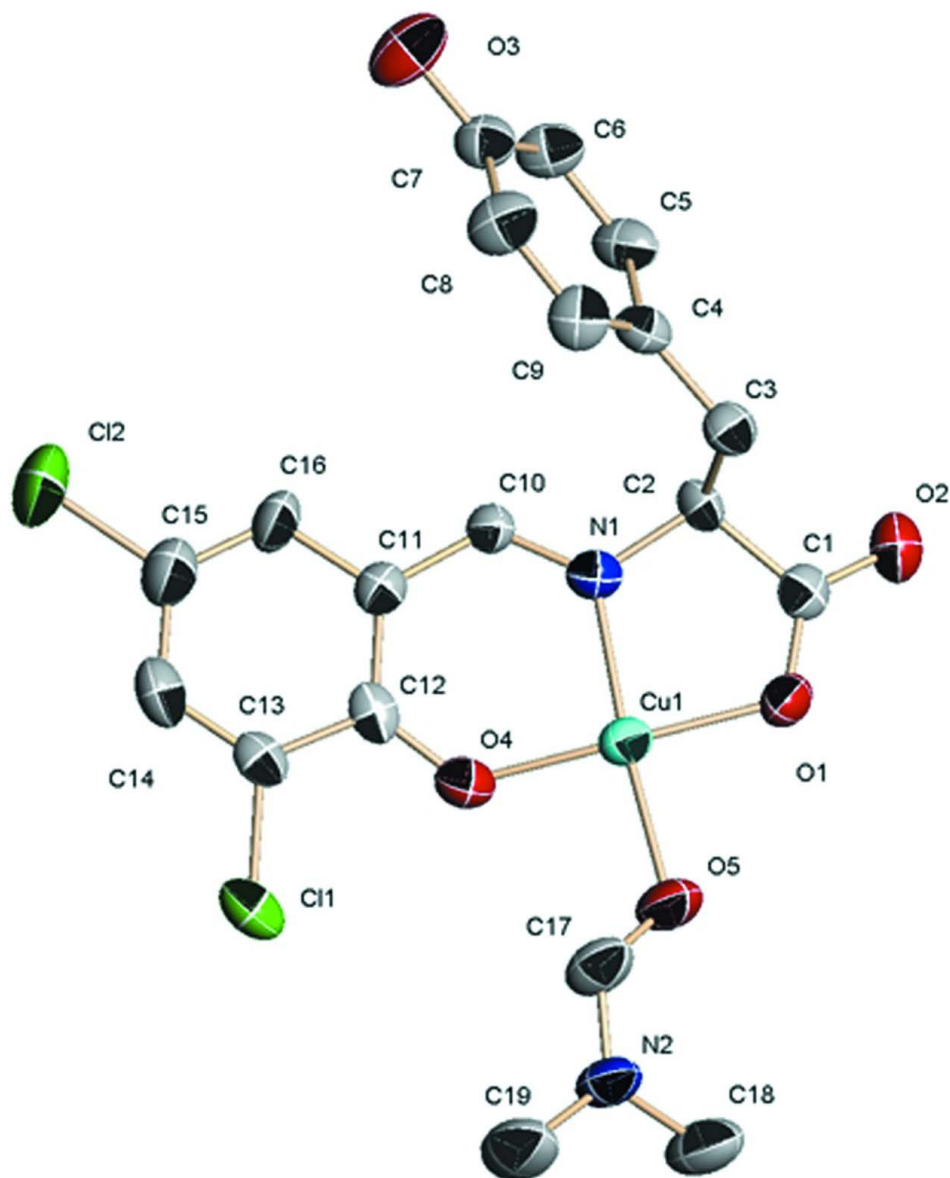


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids for non-H atoms. hydrogen atoms have been omitted.

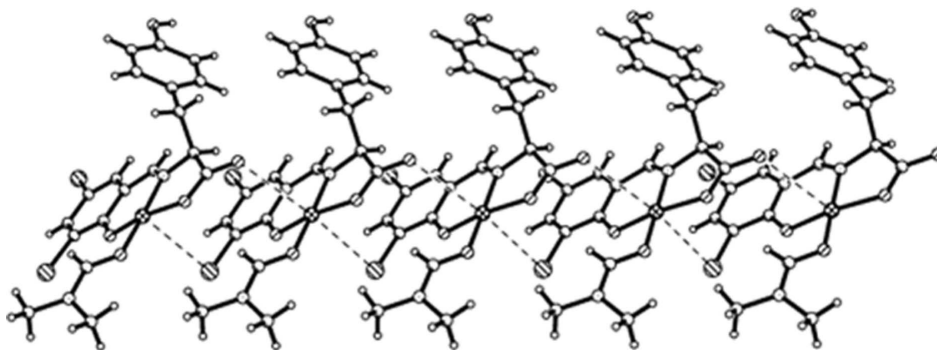


Figure 2
one-dimensional chain of (I).

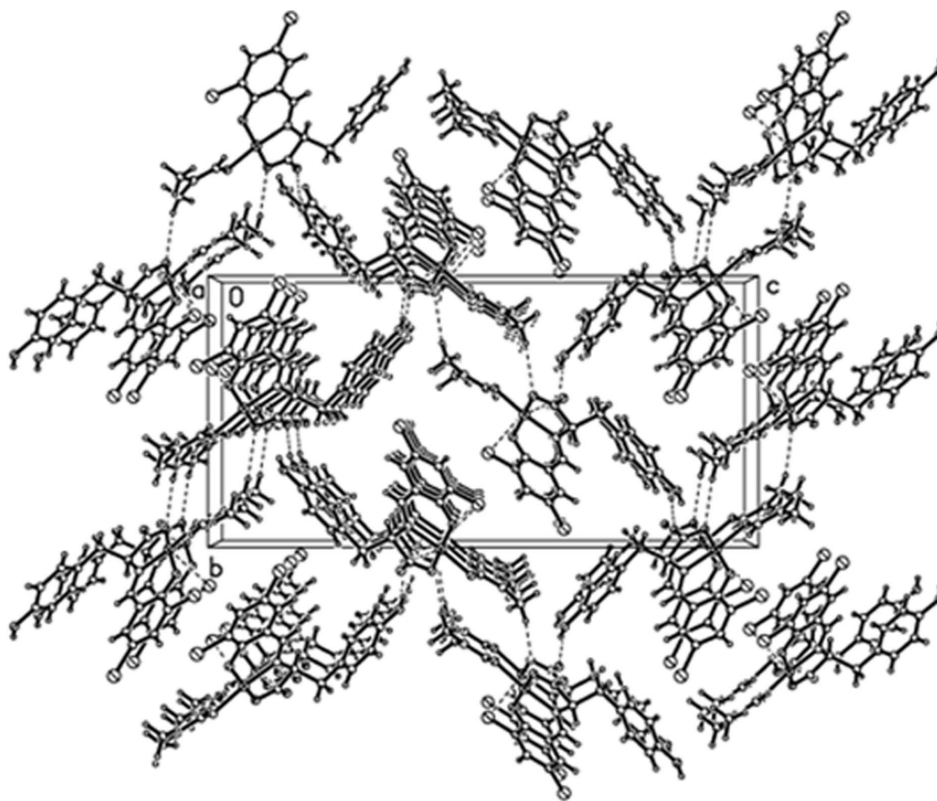


Figure 3
The three-dimensional network of (I) through hydrogen bonds.

**(2S)-[2-(3,5-Dichloro-2-oxobenzylideneamino)-3-(4-hydroxyphenyl)propionato- κ^3O,N,O']
(dimethylformamide- κO)copper(II)**

Crystal data

[Cu(C₁₆H₁₁Cl₂NO₄)(C₃H₇NO)]

$M_r = 488.79$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 5.8646$ (16) Å

$b = 13.220$ (2) Å

$c = 26.850$ (3) Å

$V = 2081.7$ (7) Å³

$Z = 4$

$F(000) = 996$

$D_x = 1.560$ Mg m⁻³

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

Cell parameters from 4089 reflections
 $\theta = 2.3\text{--}23.8^\circ$
 $\mu = 1.34 \text{ mm}^{-1}$

$T = 298 \text{ K}$
 Prism, blue
 $0.48 \times 0.20 \times 0.18 \text{ mm}$

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)
 $T_{\min} = 0.532$, $T_{\max} = 0.786$

10650 measured reflections
 3638 independent reflections
 2915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.098$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.5^\circ$
 $h = -6 \rightarrow 6$
 $k = -15 \rightarrow 12$
 $l = -31 \rightarrow 31$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.148$
 $S = 1.04$
 3638 reflections
 262 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
 $w = 1/[\sigma^2(F_o^2) + (0.0751P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.50 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983), with 1505
 Friedel pairs
 Absolute structure parameter: 0.04 (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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.87095 (14)	0.01109 (5)	0.92554 (2)	0.0398 (2)
Cl1	1.5356 (3)	0.15751 (14)	0.99080 (6)	0.0542 (5)
Cl2	1.5314 (5)	0.4447 (2)	0.84884 (10)	0.1123 (10)
N1	0.7954 (8)	0.0937 (4)	0.86843 (16)	0.0341 (12)
N2	1.2035 (10)	-0.1364 (5)	1.03525 (19)	0.0502 (15)
O1	0.5867 (8)	-0.0565 (3)	0.91109 (13)	0.0447 (11)
O2	0.2837 (8)	-0.0471 (4)	0.86065 (16)	0.0507 (12)
O3	0.9847 (9)	0.2916 (4)	0.64815 (17)	0.0663 (15)
H3	0.8857	0.3335	0.6420	0.099*
O4	1.1115 (8)	0.0946 (3)	0.94609 (13)	0.0426 (10)
O5	0.9417 (9)	-0.0841 (4)	0.97899 (16)	0.0566 (14)

C1	0.4783 (12)	-0.0227 (4)	0.8738 (2)	0.0371 (14)
C2	0.5969 (10)	0.0579 (4)	0.84153 (18)	0.0335 (13)
H2	0.4921	0.1145	0.8357	0.040*
C3	0.6629 (11)	0.0092 (4)	0.79128 (18)	0.0413 (15)
H3A	0.7794	-0.0416	0.7971	0.050*
H3B	0.5305	-0.0249	0.7776	0.050*
C4	0.7505 (11)	0.0844 (5)	0.7537 (2)	0.0390 (15)
C5	0.6177 (12)	0.1646 (5)	0.7384 (2)	0.0470 (16)
H5	0.4740	0.1726	0.7525	0.056*
C6	0.6887 (12)	0.2333 (5)	0.7032 (2)	0.0478 (18)
H6	0.5919	0.2850	0.6930	0.057*
C7	0.9055 (11)	0.2249 (5)	0.6832 (2)	0.0436 (16)
C8	1.0373 (13)	0.1453 (5)	0.6970 (2)	0.0552 (18)
H8	1.1793	0.1369	0.6822	0.066*
C9	0.9657 (12)	0.0762 (5)	0.7326 (2)	0.0477 (17)
H9	1.0625	0.0241	0.7424	0.057*
C10	0.8988 (10)	0.1759 (4)	0.85633 (19)	0.0335 (13)
H10	0.8373	0.2130	0.8301	0.040*
C11	1.1005 (11)	0.2157 (4)	0.87951 (19)	0.0367 (14)
C12	1.1995 (9)	0.1712 (4)	0.9226 (2)	0.0346 (13)
C13	1.4061 (11)	0.2142 (5)	0.93978 (19)	0.0372 (14)
C14	1.5016 (12)	0.2978 (5)	0.9188 (2)	0.0527 (18)
H14	1.6334	0.3259	0.9322	0.063*
C15	1.4005 (14)	0.3402 (5)	0.8774 (3)	0.062 (2)
C16	1.2032 (12)	0.3018 (5)	0.8584 (3)	0.0508 (18)
H16	1.1354	0.3329	0.8311	0.061*
C17	1.1375 (15)	-0.0875 (5)	0.9947 (3)	0.0558 (18)
H17	1.2486	-0.0531	0.9767	0.067*
C18	1.0416 (14)	-0.1899 (7)	1.0655 (3)	0.073 (2)
H18A	1.0066	-0.1505	1.0945	0.110*
H18B	1.1053	-0.2537	1.0754	0.110*
H18C	0.9048	-0.2013	1.0467	0.110*
C19	1.4387 (14)	-0.1337 (7)	1.0521 (3)	0.078 (3)
H19A	1.5335	-0.1067	1.0261	0.118*
H19B	1.4881	-0.2010	1.0601	0.118*
H19C	1.4502	-0.0917	1.0811	0.118*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0472 (4)	0.0363 (4)	0.0360 (3)	-0.0017 (4)	-0.0031 (3)	0.0056 (3)
Cl1	0.0510 (10)	0.0635 (11)	0.0481 (8)	0.0039 (9)	-0.0144 (7)	-0.0136 (8)
Cl2	0.117 (2)	0.0863 (18)	0.133 (2)	-0.0606 (17)	-0.0291 (18)	0.0441 (15)
N1	0.037 (3)	0.031 (3)	0.034 (2)	0.009 (2)	0.001 (2)	-0.002 (2)
N2	0.045 (3)	0.056 (4)	0.050 (3)	0.007 (3)	-0.001 (3)	0.022 (3)
O1	0.056 (3)	0.039 (2)	0.039 (2)	-0.010 (2)	0.001 (2)	0.0045 (17)
O2	0.043 (3)	0.048 (3)	0.060 (3)	-0.008 (2)	0.004 (2)	-0.009 (2)
O3	0.070 (4)	0.058 (3)	0.071 (3)	0.012 (3)	0.034 (3)	0.015 (3)

O4	0.047 (3)	0.045 (2)	0.0357 (19)	0.005 (2)	-0.003 (2)	-0.0015 (18)
O5	0.060 (4)	0.055 (3)	0.055 (3)	0.002 (3)	-0.006 (2)	0.024 (2)
C1	0.043 (4)	0.027 (3)	0.041 (3)	0.003 (3)	0.001 (3)	-0.007 (3)
C2	0.024 (3)	0.040 (3)	0.037 (3)	0.000 (3)	-0.005 (3)	-0.004 (2)
C3	0.049 (4)	0.039 (3)	0.036 (3)	-0.003 (4)	-0.003 (3)	-0.005 (3)
C4	0.043 (4)	0.040 (4)	0.034 (3)	0.005 (3)	-0.007 (3)	-0.003 (3)
C5	0.036 (3)	0.067 (4)	0.038 (3)	0.007 (4)	0.003 (3)	0.005 (3)
C6	0.046 (4)	0.050 (4)	0.047 (4)	0.015 (3)	0.003 (3)	0.007 (3)
C7	0.043 (4)	0.051 (4)	0.037 (3)	0.004 (4)	0.005 (3)	0.001 (3)
C8	0.048 (4)	0.062 (5)	0.056 (4)	0.010 (4)	0.014 (3)	0.007 (3)
C9	0.041 (4)	0.046 (4)	0.056 (4)	0.009 (3)	0.007 (3)	-0.006 (3)
C10	0.032 (3)	0.034 (3)	0.034 (3)	-0.001 (3)	0.000 (3)	0.001 (2)
C11	0.038 (4)	0.035 (3)	0.037 (3)	0.001 (3)	0.004 (3)	-0.001 (2)
C12	0.027 (3)	0.036 (3)	0.041 (3)	0.005 (3)	0.006 (3)	-0.017 (3)
C13	0.035 (4)	0.045 (4)	0.032 (3)	0.003 (3)	0.001 (3)	-0.013 (2)
C14	0.045 (4)	0.052 (4)	0.061 (4)	-0.010 (4)	-0.005 (4)	-0.015 (3)
C15	0.060 (5)	0.052 (4)	0.073 (5)	-0.013 (4)	-0.001 (4)	0.009 (4)
C16	0.050 (4)	0.038 (4)	0.064 (4)	-0.012 (3)	-0.002 (4)	0.014 (3)
C17	0.055 (5)	0.048 (4)	0.065 (4)	0.009 (4)	0.001 (4)	0.021 (3)
C18	0.063 (5)	0.093 (6)	0.064 (5)	0.001 (5)	0.003 (4)	0.038 (4)
C19	0.055 (5)	0.092 (7)	0.088 (5)	0.003 (5)	-0.017 (4)	0.037 (5)

Geometric parameters (Å, °)

Cu1—O4	1.875 (5)	C5—C6	1.374 (9)
Cu1—O1	1.931 (5)	C5—H5	0.9300
Cu1—N1	1.934 (5)	C6—C7	1.385 (9)
Cu1—O5	1.954 (4)	C6—H6	0.9300
C11—C13	1.736 (6)	C7—C8	1.357 (9)
C12—C15	1.756 (7)	C8—C9	1.387 (9)
N1—C10	1.286 (7)	C8—H8	0.9300
N1—C2	1.449 (7)	C9—H9	0.9300
N2—C17	1.324 (8)	C10—C11	1.437 (8)
N2—C18	1.435 (9)	C10—H10	0.9300
N2—C19	1.452 (9)	C11—C16	1.407 (8)
O1—C1	1.267 (7)	C11—C12	1.423 (8)
O2—C1	1.238 (7)	C12—C13	1.416 (8)
O3—C7	1.371 (7)	C13—C14	1.361 (9)
O3—H3	0.8200	C14—C15	1.379 (10)
O4—C12	1.299 (7)	C14—H14	0.9300
O5—C17	1.224 (9)	C15—C16	1.362 (10)
C1—C2	1.540 (8)	C16—H16	0.9300
C2—C3	1.545 (7)	C17—H17	0.9300
C2—H2	0.9800	C18—H18A	0.9600
C3—C4	1.508 (8)	C18—H18B	0.9600
C3—H3A	0.9700	C18—H18C	0.9600
C3—H3B	0.9700	C19—H19A	0.9600
C4—C5	1.378 (9)	C19—H19B	0.9600

C4—C9	1.387 (9)	C19—H19C	0.9600
O4—Cu1—O1	169.0 (2)	C7—C8—C9	121.8 (7)
O4—Cu1—N1	94.2 (2)	C7—C8—H8	119.1
O1—Cu1—N1	84.5 (2)	C9—C8—H8	119.1
O4—Cu1—O5	90.2 (2)	C4—C9—C8	120.3 (7)
O1—Cu1—O5	91.9 (2)	C4—C9—H9	119.9
N1—Cu1—O5	174.3 (2)	C8—C9—H9	119.9
C10—N1—C2	121.9 (5)	N1—C10—C11	126.1 (5)
C10—N1—Cu1	124.7 (4)	N1—C10—H10	117.0
C2—N1—Cu1	113.3 (4)	C11—C10—H10	117.0
C17—N2—C18	120.8 (6)	C16—C11—C12	119.2 (6)
C17—N2—C19	121.4 (7)	C16—C11—C10	118.3 (5)
C18—N2—C19	117.7 (6)	C12—C11—C10	122.5 (5)
C1—O1—Cu1	115.4 (4)	O4—C12—C13	119.7 (5)
C7—O3—H3	109.5	O4—C12—C11	123.7 (5)
C12—O4—Cu1	128.0 (4)	C13—C12—C11	116.6 (6)
C17—O5—Cu1	118.4 (5)	C14—C13—C12	122.9 (6)
O2—C1—O1	126.6 (6)	C14—C13—C11	119.8 (5)
O2—C1—C2	115.8 (5)	C12—C13—C11	117.2 (5)
O1—C1—C2	117.6 (5)	C13—C14—C15	119.2 (7)
N1—C2—C1	107.9 (4)	C13—C14—H14	120.4
N1—C2—C3	111.7 (5)	C15—C14—H14	120.4
C1—C2—C3	108.4 (5)	C16—C15—C14	121.0 (7)
N1—C2—H2	109.6	C16—C15—C12	120.1 (6)
C1—C2—H2	109.6	C14—C15—C12	118.9 (6)
C3—C2—H2	109.6	C15—C16—C11	121.0 (7)
C4—C3—C2	113.3 (5)	C15—C16—H16	119.5
C4—C3—H3A	108.9	C11—C16—H16	119.5
C2—C3—H3A	108.9	O5—C17—N2	125.2 (7)
C4—C3—H3B	108.9	O5—C17—H17	117.4
C2—C3—H3B	108.9	N2—C17—H17	117.4
H3A—C3—H3B	107.7	N2—C18—H18A	109.5
C5—C4—C9	117.0 (6)	N2—C18—H18B	109.5
C5—C4—C3	121.0 (6)	H18A—C18—H18B	109.5
C9—C4—C3	122.1 (6)	N2—C18—H18C	109.5
C6—C5—C4	122.8 (7)	H18A—C18—H18C	109.5
C6—C5—H5	118.6	H18B—C18—H18C	109.5
C4—C5—H5	118.6	N2—C19—H19A	109.5
C5—C6—C7	119.4 (6)	N2—C19—H19B	109.5
C5—C6—H6	120.3	H19A—C19—H19B	109.5
C7—C6—H6	120.3	N2—C19—H19C	109.5
C8—C7—O3	119.5 (6)	H19A—C19—H19C	109.5
C8—C7—C6	118.6 (6)	H19B—C19—H19C	109.5
O3—C7—C6	121.7 (6)		
O4—Cu1—N1—C10	-0.5 (5)	O3—C7—C8—C9	179.5 (6)
O1—Cu1—N1—C10	168.5 (5)	C6—C7—C8—C9	-3.9 (11)

O4—Cu1—N1—C2	-176.4 (4)	C5—C4—C9—C8	-1.5 (10)
O1—Cu1—N1—C2	-7.4 (3)	C3—C4—C9—C8	178.0 (6)
O4—Cu1—O1—C1	83.8 (9)	C7—C8—C9—C4	2.9 (11)
N1—Cu1—O1—C1	0.1 (4)	C2—N1—C10—C11	-177.8 (5)
O5—Cu1—O1—C1	-175.4 (4)	Cu1—N1—C10—C11	6.6 (8)
O1—Cu1—O4—C12	-90.9 (9)	N1—C10—C11—C16	174.1 (6)
N1—Cu1—O4—C12	-8.1 (5)	N1—C10—C11—C12	-5.7 (9)
O5—Cu1—O4—C12	168.2 (5)	Cu1—O4—C12—C13	-168.8 (4)
O4—Cu1—O5—C17	-26.4 (6)	Cu1—O4—C12—C11	10.8 (8)
O1—Cu1—O5—C17	164.4 (6)	C16—C11—C12—O4	176.7 (5)
Cu1—O1—C1—O2	-172.3 (5)	C10—C11—C12—O4	-3.5 (8)
Cu1—O1—C1—C2	7.0 (6)	C16—C11—C12—C13	-3.7 (8)
C10—N1—C2—C1	-164.2 (5)	C10—C11—C12—C13	176.1 (5)
Cu1—N1—C2—C1	11.9 (5)	O4—C12—C13—C14	-176.3 (5)
C10—N1—C2—C3	76.7 (7)	C11—C12—C13—C14	4.1 (8)
Cu1—N1—C2—C3	-107.2 (4)	O4—C12—C13—C11	2.3 (7)
O2—C1—C2—N1	166.9 (5)	C11—C12—C13—C11	-177.3 (4)
O1—C1—C2—N1	-12.5 (7)	C12—C13—C14—C15	-3.4 (10)
O2—C1—C2—C3	-71.9 (6)	C11—C13—C14—C15	178.1 (5)
O1—C1—C2—C3	108.7 (5)	C13—C14—C15—C16	2.2 (11)
N1—C2—C3—C4	-69.3 (6)	C13—C14—C15—C12	-177.3 (5)
C1—C2—C3—C4	171.9 (5)	C14—C15—C16—C11	-2.0 (11)
C2—C3—C4—C5	-59.0 (7)	C12—C15—C16—C11	177.5 (6)
C2—C3—C4—C9	121.5 (6)	C12—C11—C16—C15	2.8 (10)
C9—C4—C5—C6	1.3 (10)	C10—C11—C16—C15	-177.0 (6)
C3—C4—C5—C6	-178.2 (6)	Cu1—O5—C17—N2	169.3 (5)
C4—C5—C6—C7	-2.4 (10)	C18—N2—C17—O5	-1.1 (12)
C5—C6—C7—C8	3.6 (10)	C19—N2—C17—O5	-178.0 (8)
C5—C6—C7—O3	-179.8 (6)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots O2 ⁱ	0.82	1.87	2.661 (7)	163
C17—H17 \cdots O4	0.93	2.27	2.743 (8)	111
C18—H18B \cdots O1 ⁱⁱ	0.96	2.54	3.421 (10)	150

Symmetry codes: (i) $-x+1, y+1/2, -z+3/2$; (ii) $x+1/2, -y-1/2, -z+2$.