

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

{4,4'-Dichloro-2,2'-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenolato}copper(II)

 Hadi Kargar,^a Reza Kia,^{b*} Fatemeh Ganji^a and Valiollah Mirkhani^c
^aDepartment of Chemistry, Payame Noor University, PO Box 19395-3697 Tehran, I. R. of IRAN, ^bDepartment of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran, and ^cDepartment of Chemistry, University of Isfahan, 81746-73441, Isfahan, Iran

Correspondence e-mail: zsrkk@yahoo.com

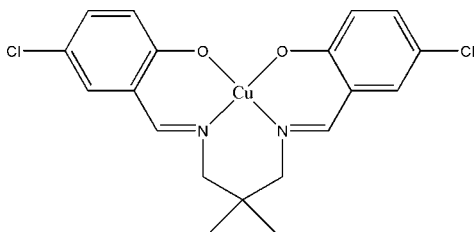
Received 20 July 2012; accepted 24 July 2012

 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.042; wR factor = 0.098; data-to-parameter ratio = 18.2.

In the title Schiff base complex, $[\text{Cu}(\text{C}_{19}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_2)]$, the Cu^{II} ion is coordinated in a distorted square-planar environment by two N atoms and two O atoms of the tetradentate ligand. The dihedral angle between the benzene rings is 36.86 (14)°. In the crystal, molecules are linked into inversion dimers by pairs of weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. In addition, $\pi-\pi$ [centroid-centroid distance = 3.7279 (16) Å] and weak $\text{C}-\text{H}\cdots\pi$ interactions are observed.

Related literature

For applications of Schiff bases in coordination chemistry, see: Granovski *et al.* (1993); Blower *et al.* (1998). For related structures, see: Ghaemi *et al.* (2011); Kargar *et al.* (2011, 2012). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

 $[\text{Cu}(\text{C}_{19}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_2)]$
 $M_r = 440.79$

 Triclinic, $P\bar{1}$
 $a = 9.4213$ (12) Å
 $b = 9.5718$ (13) Å
 $c = 11.4392$ (15) Å
 $\alpha = 74.478$ (10)°
 $\beta = 78.635$ (10)°
 $\gamma = 73.339$ (10)°

 $V = 944.1$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.46$ mm⁻¹
 $T = 296$ K
 $0.23 \times 0.12 \times 0.08$ mm

Data collection

 Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\text{min}} = 0.731$, $T_{\text{max}} = 0.893$

 8620 measured reflections
 4302 independent reflections
 3369 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.098$
 $S = 1.00$
 4302 reflections

 236 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.46$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 C_g is centroid of $\text{Cu1/O2/C17/C12/C11/N2}$.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C16}-\text{H16A}\cdots\text{O2}^{\text{i}}$	0.93	2.46	3.367 (3)	165
$\text{C10}-\text{H10B}\cdots\text{Cg}^{\text{ii}}$	0.97	2.65	3.452 (3)	140

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); 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 and PLATON (Spek, 2009).

HK and FG thanks PNU for the financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5504).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Blower, P. J. (1998). *Transition Met. Chem.*, **23**, 109–112.
- Bruker (2005). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Ghaemi, A., Rayati, S., Elahi, E., Ng, S. W. & Tiekink, E. R. T. (2011). *Acta Cryst. E* **67**, m1445–m1446.
- Granovski, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
- Kargar, H., Kia, R., Pahlavani, E. & Tahir, M. N. (2011). *Acta Cryst. E* **67**, m941.
- Kargar, H., Kia, R., Sharafi, Z. & Tahir, M. N. (2012). *Acta Cryst. E* **68**, m82.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D* **65**, 148–155.

supporting information

Acta Cryst. (2012). E68, m1135 [https://doi.org/10.1107/S1600536812033491]

{4,4'-Dichloro-2,2'-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenolato}copper(II)

Hadi Kargar, Reza Kia, Fatemeh Ganji and Valiollah Mirkhani

S1. Comment

Schiff base complexes are one of the most important stereochemical models in transition metal coordination chemistry, with ease of preparation and structural variations (Granovski *et al.*, 1993; Blower *et al.*, (1998). In continuation of our work on the crystal structure of Schiff base metal complexes (Kargar *et al.*, 2012; Kargar *et al.*, 2011; Ghaemi, *et al.*, (2011), we have determined the X-ray structure of the title compound.

The asymmetric unit of the title compound, Fig. 1, comprises a Schiff base complex. The bond lengths (Allen *et al.*, 1987) and angles are within the normal ranges and are comparable to those in related structures (Kargar *et al.*, 2012; Kargar *et al.*, 2011; Ghaemi, *et al.*, (2011).

The coordination geometry of the Cu^{II} ion is distorted square-planar which is supported by the N₂O₂ donor atoms of the coordinated Schiff base ligand. The dihedral angle between the substituted benzene rings is 36.86 (14)°. In the crystal, molecules are linked by a pair of weak C—H···O hydrogen bonds, forming inversion dimers (Table 1, Fig. 2). The crystal structure is further stabilized by intermolecular π - π interactions [$Cg1 \cdots Cg2^{iii} = 3.7279$ (16)Å; (iii) 1 - x, -y, 2 - z; Cg1 and Cg2 are centroids of the Cu1/O1/C1/C6/C7/N1 and C1-C6 rings] and C—H··· π interactions (Table 1).

S2. Experimental

The title compound was synthesized by adding 5-dichloro-salicylaldehyde-2,2-dimethyl-1, 3-propanediamine (2 mmol) to a solution of CuCl₂·4H₂O (2.1 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for half an hour. The resultant solution was filtered. Dark-green single crystals of the title compound suitable for X-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

S3. Refinement

The H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93, 0.96 and 0.97 Å for CH, CH₃ and CH₂ H-atoms, respectively, with $U_{iso}(H) = k \times U_{eq}(C)$, where $k = 1.5$ for CH₃ H-atoms, and $k = 1.2$ for all other H-atoms.

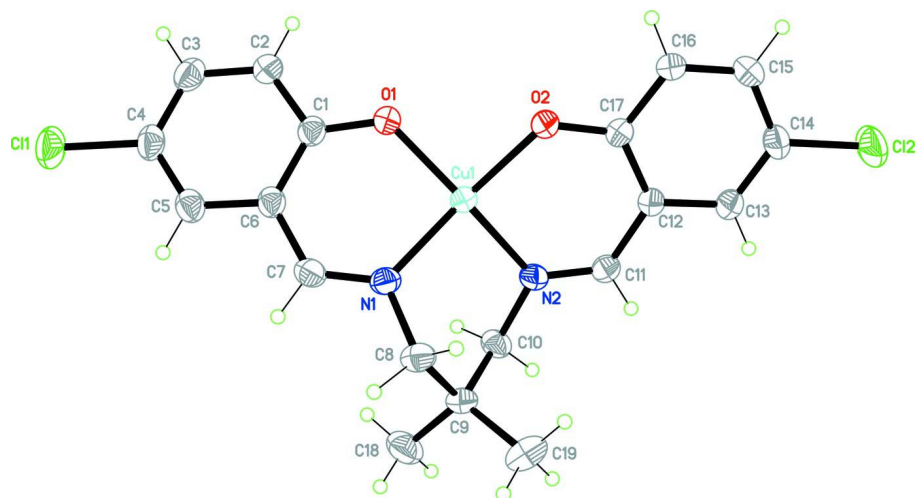


Figure 1

The molecular structure of the title compound, showing 40% probability displacement ellipsoids and the atomic numbering.

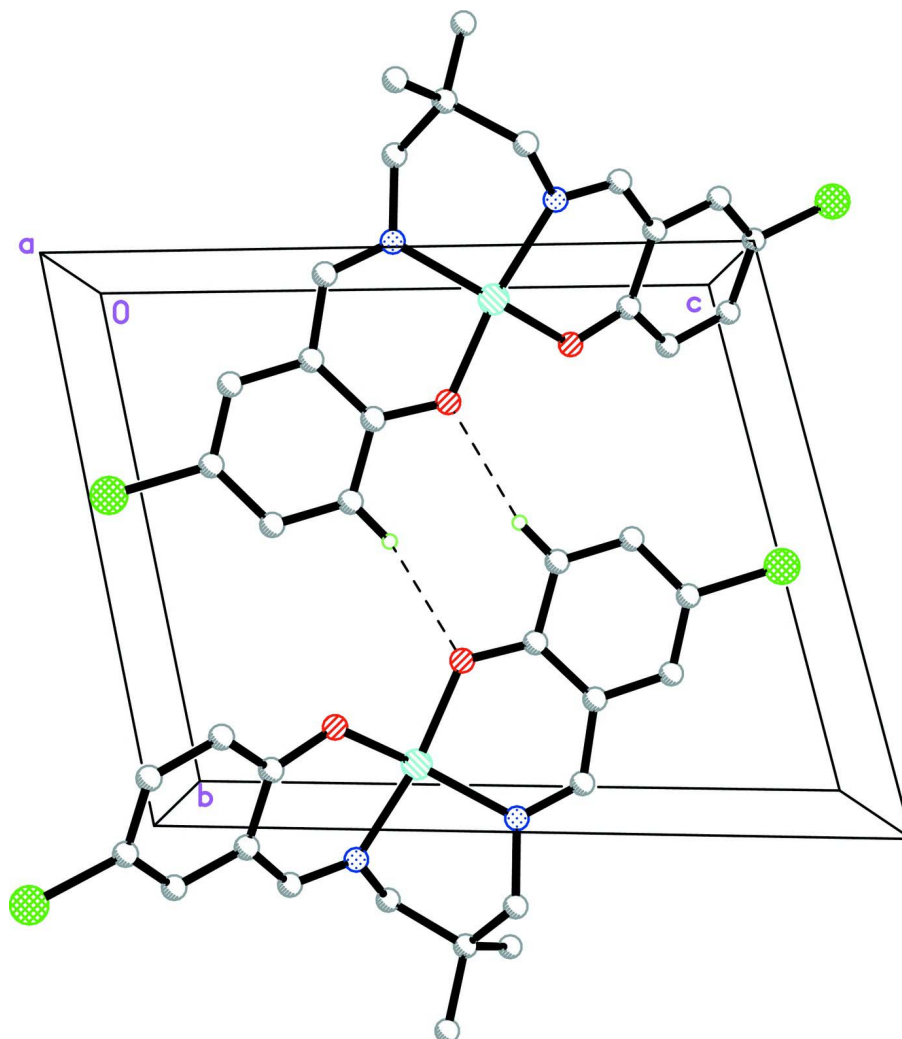


Figure 2

A part of the crystal structure of the title compound showing dimer formation through weak intermolecular C—H...O hydrogen bonds (dashed lines). Only the H atoms involved in hydrogen bonds are shown.

{4,4'-Dichloro-2,2'-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenolato}copper(II)

Crystal data

[Cu(C₁₉H₁₈Cl₂N₂O₂)]

M_r = 440.79

Triclinic, *P* $\bar{1}$

Hall symbol: -P 1

a = 9.4213 (12) Å

b = 9.5718 (13) Å

c = 11.4392 (15) Å

α = 74.478 (10)°

β = 78.635 (10)°

γ = 73.339 (10)°

V = 944.1 (2) Å³

Z = 2

F(000) = 450

D_x = 1.551 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 1540 reflections

θ = 2.5–27.4°

μ = 1.46 mm⁻¹

T = 296 K

Block, dark-green

0.23 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)

$T_{\min} = 0.731$, $T_{\max} = 0.893$

8620 measured reflections

4302 independent reflections

3369 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.098$

$S = 1.00$

4302 reflections

236 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

$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXTL* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.044 (2)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.59520 (4)	0.06692 (3)	0.63656 (3)	0.03281 (12)
Cl1	0.14886 (11)	-0.15287 (10)	1.21334 (8)	0.0638 (2)
Cl2	0.81316 (14)	0.43389 (11)	0.01358 (8)	0.0801 (3)
O1	0.4216 (2)	0.1436 (2)	0.74001 (17)	0.0395 (4)
O2	0.5916 (2)	0.2592 (2)	0.53387 (17)	0.0402 (4)
N1	0.6589 (2)	-0.1147 (2)	0.7608 (2)	0.0345 (5)
N2	0.6982 (2)	-0.0370 (2)	0.50664 (19)	0.0323 (5)
C1	0.3645 (3)	0.0694 (3)	0.8440 (2)	0.0336 (5)
C2	0.2211 (3)	0.1361 (3)	0.8969 (3)	0.0392 (6)
H2A	0.1697	0.2291	0.8560	0.047*
C3	0.1548 (3)	0.0676 (3)	1.0075 (3)	0.0439 (7)
H3A	0.0600	0.1141	1.0401	0.053*
C4	0.2299 (3)	-0.0707 (3)	1.0697 (3)	0.0427 (7)
C5	0.3678 (3)	-0.1413 (3)	1.0215 (2)	0.0401 (6)
H5A	0.4166	-0.2344	1.0641	0.048*

C6	0.4369 (3)	-0.0746 (3)	0.9079 (2)	0.0341 (5)
C7	0.5839 (3)	-0.1549 (3)	0.8646 (2)	0.0367 (6)
H7A	0.6278	-0.2433	0.9163	0.044*
C8	0.8107 (3)	-0.2035 (3)	0.7313 (3)	0.0391 (6)
H8A	0.8418	-0.2764	0.8046	0.047*
H8B	0.8782	-0.1380	0.7059	0.047*
C9	0.8246 (3)	-0.2868 (3)	0.6290 (3)	0.0370 (6)
C10	0.7130 (3)	-0.1996 (3)	0.5388 (2)	0.0365 (6)
H10A	0.7437	-0.2370	0.4645	0.044*
H10B	0.6158	-0.2182	0.5739	0.044*
C11	0.7392 (3)	0.0260 (3)	0.3960 (2)	0.0326 (5)
H11A	0.7864	-0.0363	0.3424	0.039*
C12	0.7187 (3)	0.1840 (3)	0.3477 (2)	0.0319 (5)
C13	0.7706 (3)	0.2307 (3)	0.2225 (2)	0.0388 (6)
H13A	0.8194	0.1597	0.1766	0.047*
C14	0.7498 (3)	0.3784 (3)	0.1688 (3)	0.0441 (7)
C15	0.6757 (3)	0.4870 (3)	0.2359 (3)	0.0450 (7)
H15A	0.6615	0.5880	0.1981	0.054*
C16	0.6242 (3)	0.4443 (3)	0.3570 (3)	0.0406 (6)
H16A	0.5745	0.5175	0.4005	0.049*
C17	0.6445 (3)	0.2919 (3)	0.4180 (2)	0.0333 (5)
C18	0.7882 (4)	-0.4381 (3)	0.6845 (3)	0.0563 (8)
H18A	0.7969	-0.4890	0.6206	0.084*
H18B	0.6880	-0.4233	0.7263	0.084*
H18C	0.8568	-0.4973	0.7414	0.084*
C19	0.9840 (4)	-0.3059 (4)	0.5632 (4)	0.0598 (9)
H19A	0.9953	-0.3568	0.4989	0.090*
H19B	1.0529	-0.3636	0.6203	0.090*
H19C	1.0042	-0.2093	0.5290	0.090*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03676 (19)	0.02733 (17)	0.02913 (18)	-0.00348 (12)	0.00110 (12)	-0.00637 (12)
Cl1	0.0809 (6)	0.0601 (5)	0.0447 (4)	-0.0320 (5)	0.0197 (4)	-0.0069 (4)
Cl2	0.1256 (9)	0.0540 (5)	0.0398 (4)	-0.0221 (6)	0.0211 (5)	0.0012 (4)
O1	0.0420 (10)	0.0334 (9)	0.0324 (9)	-0.0021 (8)	0.0039 (8)	-0.0038 (8)
O2	0.0512 (11)	0.0292 (9)	0.0333 (10)	-0.0068 (8)	0.0072 (8)	-0.0083 (8)
N1	0.0364 (11)	0.0319 (11)	0.0326 (11)	-0.0007 (9)	-0.0056 (9)	-0.0103 (9)
N2	0.0372 (11)	0.0254 (10)	0.0335 (11)	-0.0062 (9)	-0.0034 (9)	-0.0074 (9)
C1	0.0388 (13)	0.0343 (13)	0.0295 (12)	-0.0111 (11)	-0.0020 (11)	-0.0099 (11)
C2	0.0383 (14)	0.0366 (14)	0.0392 (14)	-0.0071 (12)	0.0007 (12)	-0.0092 (12)
C3	0.0404 (15)	0.0474 (16)	0.0446 (16)	-0.0147 (13)	0.0069 (13)	-0.0165 (14)
C4	0.0553 (17)	0.0431 (15)	0.0338 (14)	-0.0247 (14)	0.0059 (13)	-0.0103 (12)
C5	0.0530 (16)	0.0358 (14)	0.0337 (14)	-0.0167 (13)	-0.0044 (12)	-0.0064 (11)
C6	0.0408 (14)	0.0342 (13)	0.0294 (12)	-0.0124 (11)	-0.0030 (11)	-0.0083 (11)
C7	0.0449 (15)	0.0296 (12)	0.0344 (13)	-0.0042 (11)	-0.0110 (12)	-0.0065 (11)
C8	0.0360 (14)	0.0376 (14)	0.0424 (15)	-0.0007 (11)	-0.0089 (12)	-0.0128 (12)

C9	0.0375 (14)	0.0280 (12)	0.0416 (15)	-0.0014 (11)	-0.0019 (12)	-0.0106 (11)
C10	0.0464 (15)	0.0259 (12)	0.0383 (14)	-0.0102 (11)	-0.0068 (12)	-0.0071 (11)
C11	0.0346 (13)	0.0327 (12)	0.0311 (13)	-0.0070 (10)	-0.0021 (10)	-0.0114 (11)
C12	0.0323 (12)	0.0306 (12)	0.0312 (13)	-0.0085 (10)	-0.0004 (10)	-0.0065 (10)
C13	0.0440 (15)	0.0368 (14)	0.0328 (13)	-0.0098 (12)	0.0044 (12)	-0.0101 (11)
C14	0.0536 (17)	0.0414 (15)	0.0319 (14)	-0.0149 (13)	0.0013 (13)	-0.0009 (12)
C15	0.0501 (16)	0.0305 (13)	0.0462 (16)	-0.0087 (12)	-0.0009 (13)	-0.0002 (12)
C16	0.0419 (14)	0.0291 (13)	0.0425 (15)	-0.0037 (11)	0.0059 (12)	-0.0084 (11)
C17	0.0304 (12)	0.0327 (12)	0.0336 (13)	-0.0066 (10)	0.0005 (10)	-0.0067 (11)
C18	0.081 (2)	0.0308 (14)	0.0511 (18)	-0.0071 (15)	-0.0115 (17)	-0.0047 (13)
C19	0.0419 (17)	0.066 (2)	0.068 (2)	-0.0013 (16)	0.0039 (16)	-0.0295 (19)

Geometric parameters (Å, °)

Cu1—O2	1.8952 (18)	C8—H8A	0.9700
Cu1—O1	1.9050 (18)	C8—H8B	0.9700
Cu1—N2	1.952 (2)	C9—C18	1.525 (4)
Cu1—N1	1.953 (2)	C9—C19	1.525 (4)
Cl1—C4	1.749 (3)	C9—C10	1.527 (4)
Cl2—C14	1.747 (3)	C10—H10A	0.9700
O1—C1	1.312 (3)	C10—H10B	0.9700
O2—C17	1.308 (3)	C11—C12	1.434 (3)
N1—C7	1.280 (3)	C11—H11A	0.9300
N1—C8	1.466 (3)	C12—C13	1.413 (4)
N2—C11	1.283 (3)	C12—C17	1.418 (4)
N2—C10	1.471 (3)	C13—C14	1.355 (4)
C1—C2	1.411 (4)	C13—H13A	0.9300
C1—C6	1.421 (4)	C14—C15	1.398 (4)
C2—C3	1.378 (4)	C15—C16	1.367 (4)
C2—H2A	0.9300	C15—H15A	0.9300
C3—C4	1.385 (4)	C16—C17	1.414 (4)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.365 (4)	C18—H18A	0.9600
C5—C6	1.407 (4)	C18—H18B	0.9600
C5—H5A	0.9300	C18—H18C	0.9600
C6—C7	1.442 (4)	C19—H19A	0.9600
C7—H7A	0.9300	C19—H19B	0.9600
C8—C9	1.550 (4)	C19—H19C	0.9600
O2—Cu1—O1	92.08 (8)	C19—C9—C10	110.3 (3)
O2—Cu1—N2	93.57 (8)	C18—C9—C8	109.9 (2)
O1—Cu1—N2	152.81 (9)	C19—C9—C8	107.9 (2)
O2—Cu1—N1	159.03 (9)	C10—C9—C8	111.1 (2)
O1—Cu1—N1	93.46 (9)	N2—C10—C9	114.0 (2)
N2—Cu1—N1	90.69 (9)	N2—C10—H10A	108.7
C1—O1—Cu1	126.44 (16)	C9—C10—H10A	108.7
C17—O2—Cu1	127.77 (16)	N2—C10—H10B	108.7
C7—N1—C8	119.4 (2)	C9—C10—H10B	108.7

C7—N1—Cu1	125.79 (18)	H10A—C10—H10B	107.6
C8—N1—Cu1	114.63 (18)	N2—C11—C12	125.8 (2)
C11—N2—C10	119.1 (2)	N2—C11—H11A	117.1
C11—N2—Cu1	125.51 (17)	C12—C11—H11A	117.1
C10—N2—Cu1	115.01 (17)	C13—C12—C17	120.0 (2)
O1—C1—C2	118.3 (2)	C13—C12—C11	116.9 (2)
O1—C1—C6	124.7 (2)	C17—C12—C11	123.1 (2)
C2—C1—C6	117.0 (2)	C14—C13—C12	120.4 (2)
C3—C2—C1	122.0 (3)	C14—C13—H13A	119.8
C3—C2—H2A	119.0	C12—C13—H13A	119.8
C1—C2—H2A	119.0	C13—C14—C15	120.7 (3)
C2—C3—C4	119.7 (3)	C13—C14—C12	119.7 (2)
C2—C3—H3A	120.1	C15—C14—C12	119.6 (2)
C4—C3—H3A	120.1	C16—C15—C14	119.9 (3)
C5—C4—C3	120.6 (3)	C16—C15—H15A	120.1
C5—C4—C11	119.9 (2)	C14—C15—H15A	120.1
C3—C4—C11	119.5 (2)	C15—C16—C17	121.8 (2)
C4—C5—C6	120.7 (3)	C15—C16—H16A	119.1
C4—C5—H5A	119.6	C17—C16—H16A	119.1
C6—C5—H5A	119.6	O2—C17—C16	118.5 (2)
C5—C6—C1	119.9 (2)	O2—C17—C12	124.3 (2)
C5—C6—C7	117.3 (2)	C16—C17—C12	117.2 (2)
C1—C6—C7	122.8 (2)	C9—C18—H18A	109.5
N1—C7—C6	125.4 (2)	C9—C18—H18B	109.5
N1—C7—H7A	117.3	H18A—C18—H18B	109.5
C6—C7—H7A	117.3	C9—C18—H18C	109.5
N1—C8—C9	113.3 (2)	H18A—C18—H18C	109.5
N1—C8—H8A	108.9	H18B—C18—H18C	109.5
C9—C8—H8A	108.9	C9—C19—H19A	109.5
N1—C8—H8B	108.9	C9—C19—H19B	109.5
C9—C8—H8B	108.9	H19A—C19—H19B	109.5
H8A—C8—H8B	107.7	C9—C19—H19C	109.5
C18—C9—C19	111.0 (3)	H19A—C19—H19C	109.5
C18—C9—C10	106.7 (2)	H19B—C19—H19C	109.5
O2—Cu1—O1—C1	-172.8 (2)	C8—N1—C7—C6	176.8 (2)
N2—Cu1—O1—C1	85.3 (3)	Cu1—N1—C7—C6	1.2 (4)
N1—Cu1—O1—C1	-13.0 (2)	C5—C6—C7—N1	176.0 (2)
O1—Cu1—O2—C17	-153.3 (2)	C1—C6—C7—N1	-7.1 (4)
N2—Cu1—O2—C17	0.1 (2)	C7—N1—C8—C9	111.5 (3)
N1—Cu1—O2—C17	101.4 (3)	Cu1—N1—C8—C9	-72.4 (3)
O2—Cu1—N1—C7	112.0 (3)	N1—C8—C9—C18	-87.2 (3)
O1—Cu1—N1—C7	6.9 (2)	N1—C8—C9—C19	151.7 (3)
N2—Cu1—N1—C7	-146.2 (2)	N1—C8—C9—C10	30.7 (3)
O2—Cu1—N1—C8	-63.9 (3)	C11—N2—C10—C9	114.9 (3)
O1—Cu1—N1—C8	-168.88 (17)	Cu1—N2—C10—C9	-71.5 (3)
N2—Cu1—N1—C8	38.01 (18)	C18—C9—C10—N2	161.2 (2)
O2—Cu1—N2—C11	0.1 (2)	C19—C9—C10—N2	-78.2 (3)

O1—Cu1—N2—C11	101.7 (3)	C8—C9—C10—N2	41.4 (3)
N1—Cu1—N2—C11	-159.3 (2)	C10—N2—C11—C12	173.6 (2)
O2—Cu1—N2—C10	-172.92 (17)	Cu1—N2—C11—C12	0.8 (4)
O1—Cu1—N2—C10	-71.3 (3)	N2—C11—C12—C13	-179.3 (3)
N1—Cu1—N2—C10	27.62 (18)	N2—C11—C12—C17	-2.0 (4)
Cu1—O1—C1—C2	-168.66 (18)	C17—C12—C13—C14	-0.1 (4)
Cu1—O1—C1—C6	11.3 (4)	C11—C12—C13—C14	177.2 (3)
O1—C1—C2—C3	-178.2 (2)	C12—C13—C14—C15	-0.5 (5)
C6—C1—C2—C3	1.8 (4)	C12—C13—C14—C12	-179.4 (2)
C1—C2—C3—C4	0.2 (4)	C13—C14—C15—C16	0.3 (5)
C2—C3—C4—C5	-1.3 (4)	C12—C14—C15—C16	179.2 (2)
C2—C3—C4—C11	177.0 (2)	C14—C15—C16—C17	0.5 (5)
C3—C4—C5—C6	0.4 (4)	Cu1—O2—C17—C16	177.33 (19)
C11—C4—C5—C6	-177.9 (2)	Cu1—O2—C17—C12	-1.2 (4)
C4—C5—C6—C1	1.7 (4)	C15—C16—C17—O2	-179.7 (3)
C4—C5—C6—C7	178.7 (2)	C15—C16—C17—C12	-1.0 (4)
O1—C1—C6—C5	177.4 (2)	C13—C12—C17—O2	179.4 (2)
C2—C1—C6—C5	-2.7 (4)	C11—C12—C17—O2	2.2 (4)
O1—C1—C6—C7	0.5 (4)	C13—C12—C17—C16	0.8 (4)
C2—C1—C6—C7	-179.6 (2)	C11—C12—C17—C16	-176.3 (2)

Hydrogen-bond geometry (Å, °)

C_g is centroid of Cu1/O2/C17/C12/C11/N2.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C16—H16 <i>A</i> ...O2 ⁱ	0.93	2.46	3.367 (3)	165
C10—H10 <i>B</i> ...C _g ⁱⁱ	0.97	2.65	3.452 (3)	140

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