

Chlorido(4-methylpyridin-2-amine- κN^1)-(2-[[[(4-methylpyridin-2-yl)imino- κN]-methyl]phenolato- κO]copper(II)

 Bussa Bhagyaraju, P. Sambasiva Rao[‡] and Toka Swu*

Department of Chemistry, Pondicherry University, R.V. Nagar, Kalapet, Puducherry 605 014, India

Correspondence e-mail: tokaswu.che@pondiuni.edu.in

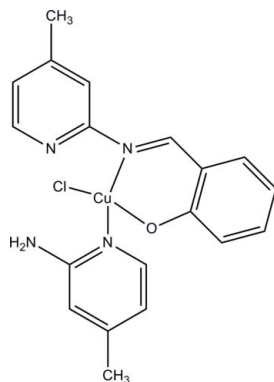
Received 25 October 2012; accepted 16 November 2012

 Key indicators: single-crystal X-ray study; $T = 300$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.055; wR factor = 0.114; data-to-parameter ratio = 13.7.

In the title complex, $[Cu(C_{13}H_{11}N_2O)Cl(C_6H_8N_2)]$, the Cu^{II} atom adopts a distorted tetrahedral geometry being coordinated by the phenolic O atom and the azomethine N atom of the Schiff base ligand *N*-salicylidene 2-aminopyridine, and by the 2-aminopyridine N atom and a Cl atom. The pyridyl N atom of the Schiff base and the imino N atom of the 4-methylpyridine-2-ylimino ligand are not involved in the coordination. There is an intramolecular $N-H \cdots N$ hydrogen bond involving the pyridine N atom and the amino group of the 2-aminopyridine ligand. In the crystal, molecules are linked *via* $N-H \cdots Cl$ hydrogen bonds, forming chains propagating along [001].

Related literature

For the preparation of similar compounds, see: Miao *et al.* (2009); Parashar *et al.* (1988); Castineiras *et al.* (1989). For the crystal structures of related compounds, see: Castineiras *et al.* (1989); Miao *et al.* (2009).


[‡] Deceased.

Experimental

Crystal data

$[Cu(C_{13}H_{11}N_2O)Cl(C_6H_8N_2)]$	$V = 1846.1 (6) \text{ \AA}^3$
$M_r = 418.37$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 17.443 (4) \text{ \AA}$	$\mu = 1.34 \text{ mm}^{-1}$
$b = 11.2197 (19) \text{ \AA}$	$T = 300 \text{ K}$
$c = 9.4435 (19) \text{ \AA}$	$0.40 \times 0.40 \times 0.06 \text{ mm}$
$\beta = 92.67 (2)^\circ$	

Data collection

Oxford Diffraction Xcalibur, Eos diffractometer	7213 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2010)	3339 independent reflections
$T_{\min} = 0.565$, $T_{\max} = 1.000$	2017 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.114$	$\Delta\rho_{\max} = 0.40 \text{ e \AA}^{-3}$
$S = 0.94$	$\Delta\rho_{\min} = -0.45 \text{ e \AA}^{-3}$
3339 reflections	
243 parameters	
2 restraints	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2NB \cdots N3$	0.85 (4)	2.27 (4)	3.039 (6)	150 (5)
$N2-H2NA \cdots Cl1^i$	0.86 (4)	2.44 (4)	3.305 (5)	179 (7)

 Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2009); software used to prepare material for publication: *OLEX2*.

BB thanks the Department of Science and Technology, New Delhi, India, for financial support and for providing the single-crystal X-ray diffractometer facility at the Department of Chemistry, Pondicherry University, under the DST-FIST program.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2518).

References

- Castineiras, A., Castro, J. A., Duran, M. L., Garcia-Vazquez, J. A., Romero, J. & Sousa, A. (1989). *Polyhedron*, **8**, 2543–2549.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Miao, J., Zhao, Z., Chen, H., Wang, D. & Nie, Y. (2009). *Acta Cryst.* **E65**, m904.
- Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd., Yarnton, England.
- Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supplementary materials

Acta Cryst. (2012). E68, m1523 [doi:10.1107/S1600536812047198]

Chlorido(4-methylpyridin-2-amine- κN^1)(2-[(4-methylpyridin-2-yl)imino- κN]methyl}phenolato- κO)copper(II)

Bussa Bhagyaraju, P. Sambasiva Rao and Toka Swu

Comment

The Schiff base, *N*-salicylidene 2-aminopyridine, has been widely studied as a potential tridentate ligand. For example, the complex Bis{2-[(2-pyridyl)iminomethyl]-phenolato}copper(II), has been prepared by (Miao *et al.*, 2009), who reported that to a green solution of salicylaldehyde (0.19 mmol) and Cu(OAc)₂·H₂O (0.05 mmol) in ethanol they added slowly an ethanolic solution of 2-aminopyridine (0.22 mmol). The resulting mixture was allowed to stand and brown crystalline needles were obtained after 1 day. The same compound was prepared by an electrochemical method (Castineiras *et al.*, 1989) and by a solution method (Parashar *et al.*, 1988). We have used same procedure as (Miao *et al.*, 2009), but using a 1:1:1 molar ratio that produced the yellow crystals of the title compound, whose crystal structure we report on herein.

In the title complex, Fig. 1, the copper atom has a slightly distorted tetrahedral geometry. It coordinates to the phenolic atom O1 and the azomethine atom N4 of the Schiff base ligand *N*-salicylidene 2-aminopyridine, and to the 2-aminopyridine atom N1 and a chlorine atom, Cl1. The Cu—O1 and Cu—N4 bond lengths are similar to those reported in related structures (Miao *et al.*, 2009; Castineiras *et al.*, 1989). The structure of the molecule is stabilized by an intramolecular N—H...Cl hydrogen bond (Table 1).

In the crystal, the intermolecular N—H...Cl hydrogen bond (Fig. 2 and Table 1) plays an important role in linking the molecules to form chains propagating along the *c* axis, as shown in Fig. 3.

Experimental

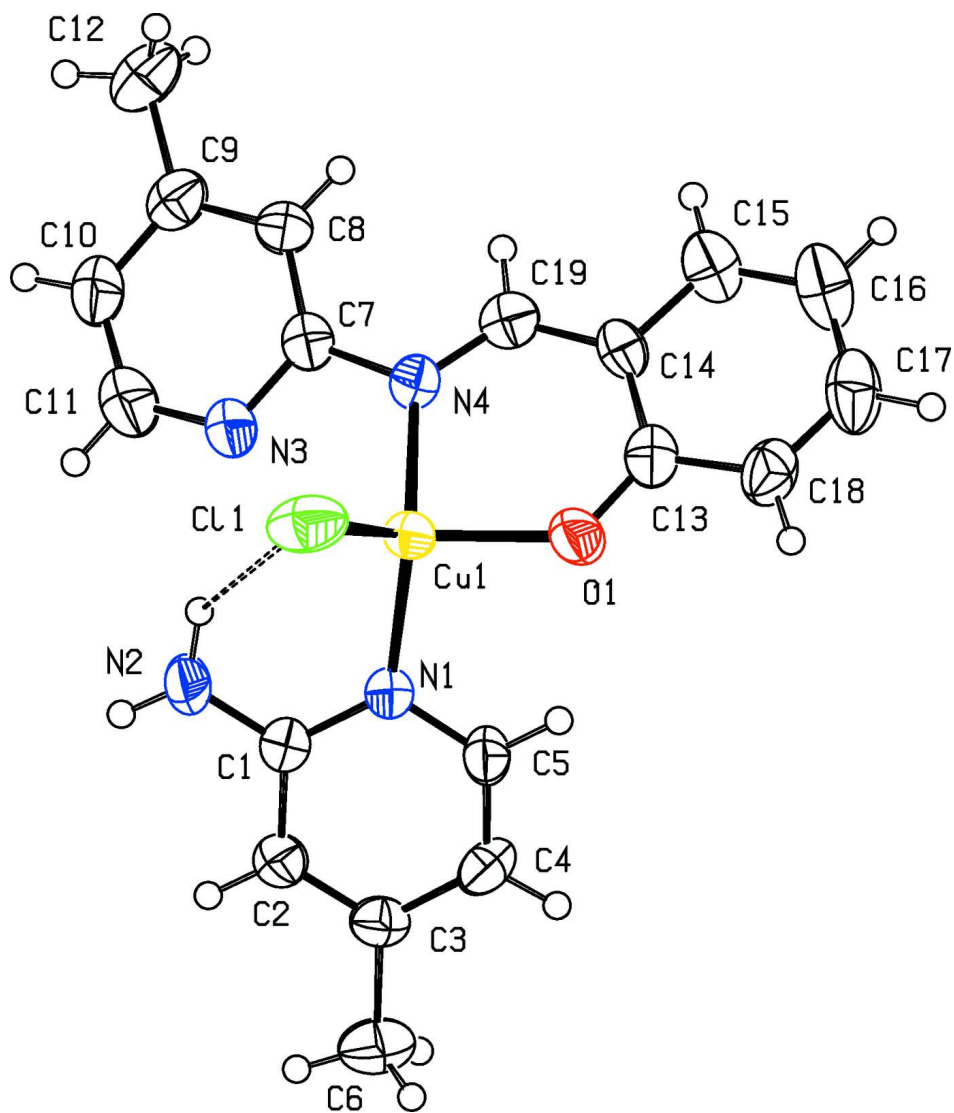
A methanolic solution of 2-(((4-methyl-pyridine-2-yl)imino)methyl)phenol (0.01 moles) and 4-methylpyridin-2-amine (0.01 moles) was added slowly to a methanolic solution of copper chloride (0.01 moles). The resulting mixture was allowed to stand and yellow plate-like crystals were obtained after ca. 7 days.

Refinement

The NH₂ H-atoms were located in a difference Fourier map and refined with distances restraints: N—H = 0.86 (2) Å. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.93 and 0.96 Å, for CH and CH₃ H atoms, respectively; $U_{iso} = k \times U_{eq}(N,C)$, where $k = 1.5$ for CH₃ H atoms, and = 1.2 for other H atoms.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

**Figure 1**

The molecular structure of title compound, showing the atom numbering. The displacement ellipsoids are drawn at the 50% probability level. The intramolecular N-H...Cl bond is shown as a dashed line (see Table 1 for details).

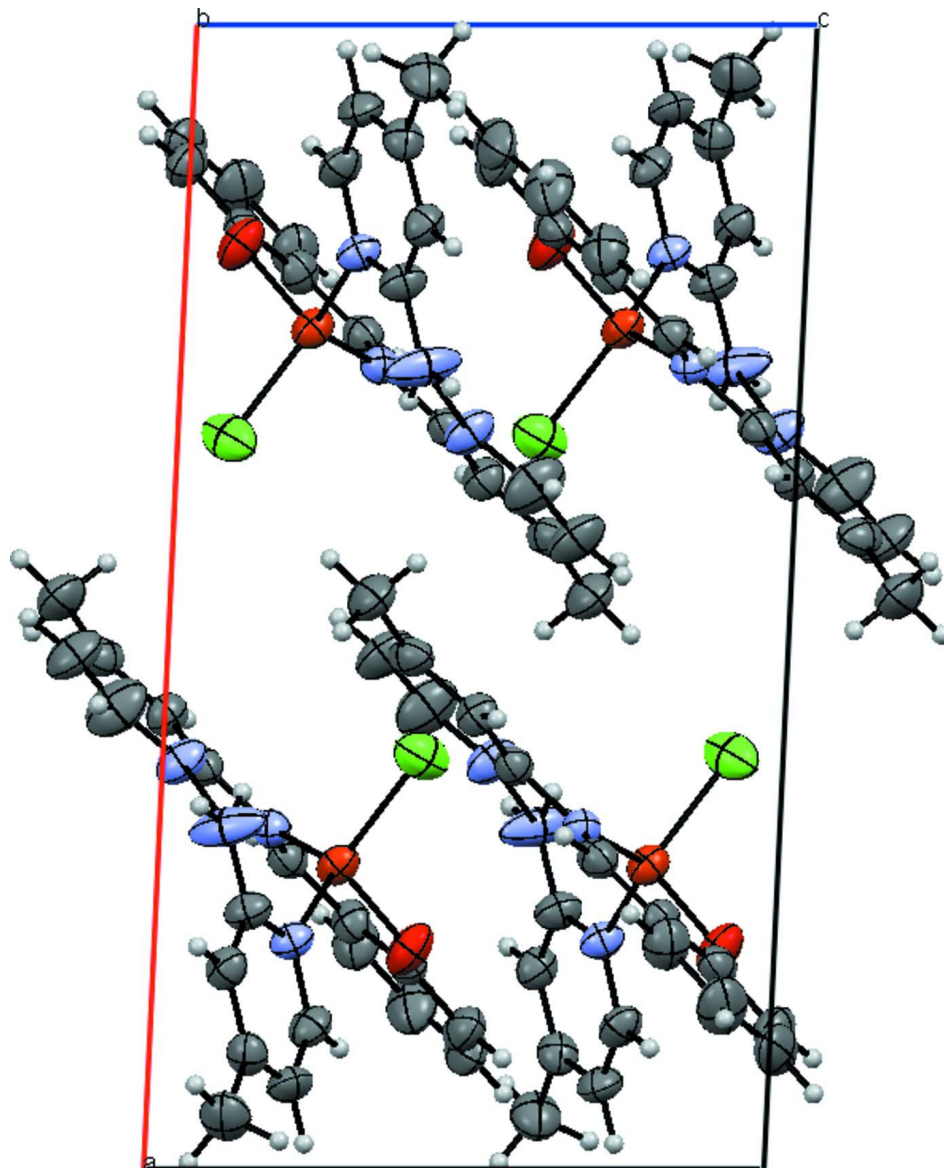
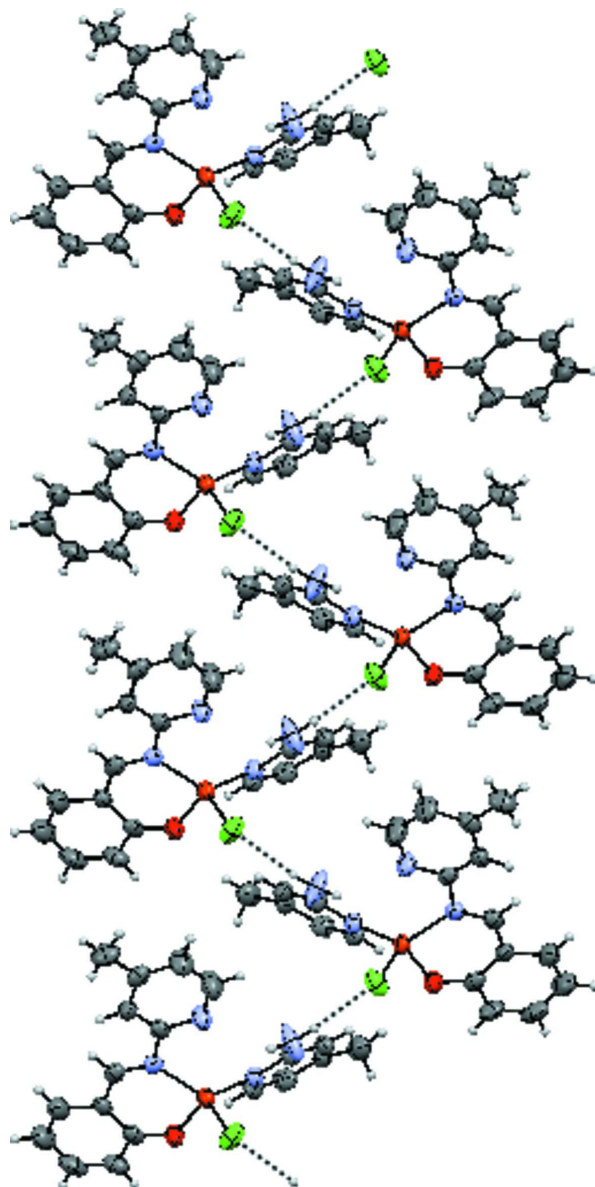


Figure 2

A view along *b* axis of the crystal packing of the title compound.

**Figure 3**

A view of the N-H...Cl hydrogen bonded chain structure propagating along the *c* axis direction (dashed line; see Table 1 for details).

Chlorido(4-methylpyridin-2-amine- κN^1)(2-[[4-methylpyridin-2-yl]imino- κN]methyl)phenolato- κO)copper(II)

Crystal data

[Cu(C₁₃H₁₁N₂O)Cl(C₆H₈N₂)]

$M_r = 418.37$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 17.443 (4) \text{ \AA}$

$b = 11.2197 (19) \text{ \AA}$

$c = 9.4435 (19) \text{ \AA}$

$\beta = 92.67 (2)^\circ$

$V = 1846.1 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 860$

$D_x = 1.505 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71070 \text{ \AA}$

Cell parameters from 2251 reflections

$\theta = 2.8\text{--}29.4^\circ$

$\mu = 1.34 \text{ mm}^{-1}$

$T = 300$ K
Plate, yellow

$0.4 \times 0.4 \times 0.06$ mm

Data collection

Oxford Diffraction Xcalibur, Eos diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
 ω scans
Absorption correction: multi-scan
(*CrysAlis PRO*; Oxford Diffraction, 2010)
 $T_{\min} = 0.565$, $T_{\max} = 1.000$

7213 measured reflections
3339 independent reflections
2017 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$
 $\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -14 \rightarrow 20$
 $k = -13 \rightarrow 10$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.114$
 $S = 0.94$
3339 reflections
243 parameters
2 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0352P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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	0.23453 (3)	0.51797 (4)	0.79066 (6)	0.0389 (2)
Cl1	0.13907 (8)	0.44704 (11)	0.91654 (15)	0.0642 (5)
O1	0.30823 (19)	0.6041 (3)	0.9125 (3)	0.0528 (13)
N1	0.3004 (2)	0.3846 (3)	0.7218 (4)	0.0385 (12)
N2	0.2006 (3)	0.2818 (4)	0.6107 (6)	0.079 (2)
N3	0.1439 (2)	0.5299 (3)	0.5301 (5)	0.0526 (16)
N4	0.2022 (2)	0.6618 (3)	0.6805 (4)	0.0367 (12)
C1	0.2746 (3)	0.2872 (4)	0.6490 (5)	0.0436 (17)
C2	0.3246 (3)	0.1932 (4)	0.6186 (5)	0.0432 (17)
C3	0.3996 (3)	0.1993 (4)	0.6589 (5)	0.0420 (17)
C4	0.4263 (3)	0.3013 (4)	0.7295 (5)	0.0476 (17)
C5	0.3758 (3)	0.3887 (4)	0.7583 (5)	0.0433 (17)
C6	0.4539 (3)	0.0991 (4)	0.6281 (5)	0.061 (2)
C7	0.1478 (3)	0.6438 (4)	0.5666 (5)	0.0389 (17)
C8	0.1030 (3)	0.7309 (4)	0.5036 (5)	0.0424 (17)

C9	0.0524 (3)	0.7024 (4)	0.3933 (5)	0.0476 (17)
C10	0.0505 (3)	0.5841 (4)	0.3494 (6)	0.067 (2)
C11	0.0968 (4)	0.5026 (5)	0.4217 (7)	0.077 (3)
C12	0.0006 (3)	0.7932 (5)	0.3246 (6)	0.066 (2)
C13	0.3222 (3)	0.7167 (4)	0.9098 (5)	0.0421 (17)
C14	0.2837 (3)	0.7994 (4)	0.8159 (5)	0.0406 (17)
C15	0.3030 (3)	0.9213 (4)	0.8254 (5)	0.0577 (19)
C16	0.3574 (4)	0.9616 (5)	0.9200 (6)	0.072 (3)
C17	0.3958 (3)	0.8815 (5)	1.0102 (6)	0.066 (2)
C18	0.3778 (3)	0.7637 (4)	1.0062 (5)	0.053 (2)
C19	0.2287 (3)	0.7673 (4)	0.7090 (5)	0.0428 (17)
H2NA	0.184 (3)	0.223 (3)	0.559 (5)	0.0950*
H2	0.30570	0.12630	0.57040	0.0520*
H2NB	0.177 (3)	0.348 (3)	0.618 (6)	0.0950*
H4	0.47800	0.30930	0.75630	0.0570*
H5	0.39440	0.45580	0.80650	0.0520*
H6A	0.42650	0.03750	0.57640	0.0920*
H6B	0.47520	0.06720	0.71560	0.0920*
H6C	0.49450	0.12870	0.57260	0.0920*
H8	0.10680	0.80920	0.53560	0.0510*
H10	0.01860	0.56040	0.27290	0.0800*
H11	0.09480	0.42360	0.39210	0.0930*
H12A	-0.02900	0.83080	0.39510	0.0990*
H12B	-0.03320	0.75510	0.25550	0.0990*
H12C	0.03080	0.85210	0.27880	0.0990*
H15	0.27770	0.97530	0.76500	0.0700*
H16	0.36900	1.04250	0.92470	0.0850*
H17	0.43420	0.90870	1.07380	0.0780*
H18	0.40330	0.71230	1.06970	0.0640*
H19	0.20910	0.82900	0.65230	0.0520*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0416 (4)	0.0315 (3)	0.0429 (4)	0.0040 (3)	-0.0052 (3)	-0.0010 (3)
Cl1	0.0576 (10)	0.0592 (8)	0.0768 (10)	0.0139 (7)	0.0154 (8)	0.0244 (8)
O1	0.067 (3)	0.0363 (18)	0.053 (2)	0.0006 (16)	-0.0208 (19)	-0.0021 (17)
N1	0.035 (2)	0.034 (2)	0.046 (2)	-0.0017 (18)	-0.004 (2)	-0.0007 (19)
N2	0.043 (3)	0.052 (3)	0.139 (5)	0.006 (2)	-0.026 (3)	-0.049 (3)
N3	0.053 (3)	0.041 (2)	0.062 (3)	-0.003 (2)	-0.016 (2)	-0.006 (2)
N4	0.034 (2)	0.040 (2)	0.036 (2)	-0.0026 (18)	0.0004 (19)	0.0008 (19)
C1	0.037 (3)	0.040 (3)	0.053 (3)	-0.001 (2)	-0.005 (3)	-0.003 (3)
C2	0.045 (3)	0.040 (3)	0.044 (3)	0.003 (2)	-0.003 (3)	-0.005 (2)
C3	0.046 (3)	0.039 (3)	0.041 (3)	0.008 (2)	0.003 (3)	-0.001 (2)
C4	0.033 (3)	0.060 (3)	0.049 (3)	0.008 (3)	-0.006 (3)	0.000 (3)
C5	0.042 (3)	0.041 (3)	0.046 (3)	-0.008 (2)	-0.009 (3)	-0.003 (2)
C6	0.060 (4)	0.061 (3)	0.063 (4)	0.021 (3)	0.008 (3)	0.001 (3)
C7	0.038 (3)	0.042 (3)	0.037 (3)	-0.004 (2)	0.006 (2)	-0.004 (2)
C8	0.045 (3)	0.037 (3)	0.045 (3)	0.001 (2)	-0.001 (3)	0.005 (2)
C9	0.037 (3)	0.055 (3)	0.051 (3)	-0.003 (3)	0.004 (3)	0.015 (3)

C10	0.062 (4)	0.059 (4)	0.077 (4)	-0.010 (3)	-0.026 (3)	-0.006 (3)
C11	0.084 (5)	0.053 (3)	0.092 (5)	-0.005 (3)	-0.027 (4)	-0.015 (3)
C12	0.053 (4)	0.086 (4)	0.058 (4)	0.008 (3)	-0.011 (3)	0.013 (3)
C13	0.038 (3)	0.051 (3)	0.038 (3)	-0.005 (2)	0.008 (3)	-0.009 (3)
C14	0.048 (3)	0.037 (3)	0.037 (3)	-0.006 (2)	0.004 (3)	-0.009 (2)
C15	0.069 (4)	0.051 (3)	0.053 (3)	-0.014 (3)	0.002 (3)	-0.003 (3)
C16	0.084 (5)	0.068 (4)	0.062 (4)	-0.030 (4)	-0.001 (4)	-0.011 (3)
C17	0.065 (4)	0.083 (4)	0.049 (4)	-0.019 (3)	0.001 (3)	-0.026 (3)
C18	0.049 (4)	0.067 (4)	0.043 (3)	0.002 (3)	-0.008 (3)	-0.014 (3)
C19	0.041 (3)	0.046 (3)	0.042 (3)	0.001 (2)	0.007 (3)	0.005 (3)

Geometric parameters (Å, °)

Cu1—C11	2.2368 (16)	C13—C18	1.402 (7)
Cu1—O1	1.942 (3)	C13—C14	1.429 (7)
Cu1—N1	2.013 (4)	C14—C19	1.407 (7)
Cu1—N3	2.865 (5)	C14—C15	1.410 (6)
Cu1—N4	1.987 (4)	C15—C16	1.351 (8)
O1—C13	1.287 (6)	C16—C17	1.389 (8)
N1—C1	1.357 (6)	C17—C18	1.359 (7)
N1—C5	1.345 (6)	C2—H2	0.9300
N2—C1	1.326 (7)	C4—H4	0.9300
N3—C7	1.325 (6)	C5—H5	0.9300
N3—C11	1.319 (8)	C6—H6A	0.9600
N4—C7	1.415 (6)	C6—H6B	0.9600
N4—C19	1.295 (6)	C6—H6C	0.9600
N2—H2NB	0.85 (4)	C8—H8	0.9300
N2—H2NA	0.86 (4)	C10—H10	0.9300
C1—C2	1.407 (7)	C11—H11	0.9300
C2—C3	1.347 (7)	C12—H12A	0.9600
C3—C6	1.507 (7)	C12—H12B	0.9600
C3—C4	1.394 (7)	C12—H12C	0.9600
C4—C5	1.354 (7)	C15—H15	0.9300
C7—C8	1.370 (7)	C16—H16	0.9300
C8—C9	1.371 (7)	C17—H17	0.9300
C9—C10	1.391 (6)	C18—H18	0.9300
C9—C12	1.490 (7)	C19—H19	0.9300
C10—C11	1.380 (8)		
C11—Cu1—O1	110.53 (10)	C14—C13—C18	116.7 (4)
C11—Cu1—N1	110.94 (11)	C13—C14—C15	119.1 (4)
C11—Cu1—N3	94.50 (9)	C13—C14—C19	124.3 (4)
C11—Cu1—N4	111.53 (11)	C15—C14—C19	116.5 (4)
O1—Cu1—N1	100.91 (14)	C14—C15—C16	121.7 (5)
O1—Cu1—N3	144.00 (12)	C15—C16—C17	119.5 (5)
O1—Cu1—N4	94.01 (14)	C16—C17—C18	120.6 (5)
N1—Cu1—N3	93.31 (13)	C13—C18—C17	122.4 (5)
N1—Cu1—N4	125.93 (15)	N4—C19—C14	127.5 (4)
N3—Cu1—N4	51.74 (13)	C1—C2—H2	120.00
Cu1—O1—C13	126.7 (3)	C3—C2—H2	120.00

Cu1—N1—C1	125.6 (3)	C3—C4—H4	121.00
Cu1—N1—C5	117.3 (3)	C5—C4—H4	120.00
C1—N1—C5	117.1 (4)	N1—C5—H5	118.00
Cu1—N3—C7	78.6 (3)	C4—C5—H5	118.00
Cu1—N3—C11	162.7 (3)	C3—C6—H6A	109.00
C7—N3—C11	116.7 (4)	C3—C6—H6B	109.00
Cu1—N4—C7	116.5 (3)	C3—C6—H6C	109.00
Cu1—N4—C19	122.9 (3)	H6A—C6—H6B	109.00
C7—N4—C19	120.6 (4)	H6A—C6—H6C	109.00
H2NA—N2—H2NB	124 (5)	H6B—C6—H6C	109.00
C1—N2—H2NB	114 (3)	C7—C8—H8	120.00
C1—N2—H2NA	119 (3)	C9—C8—H8	120.00
N2—C1—C2	121.0 (4)	C9—C10—H10	121.00
N1—C1—N2	118.1 (4)	C11—C10—H10	121.00
N1—C1—C2	120.9 (5)	N3—C11—H11	118.00
C1—C2—C3	120.5 (4)	C10—C11—H11	118.00
C2—C3—C4	118.4 (4)	C9—C12—H12A	109.00
C2—C3—C6	121.2 (4)	C9—C12—H12B	109.00
C4—C3—C6	120.4 (5)	C9—C12—H12C	109.00
C3—C4—C5	119.0 (5)	H12A—C12—H12B	110.00
N1—C5—C4	124.2 (4)	H12A—C12—H12C	110.00
N3—C7—C8	123.6 (5)	H12B—C12—H12C	109.00
N3—C7—N4	111.1 (4)	C14—C15—H15	119.00
N4—C7—C8	125.2 (4)	C16—C15—H15	119.00
C7—C8—C9	119.8 (4)	C15—C16—H16	120.00
C8—C9—C10	117.0 (4)	C17—C16—H16	120.00
C10—C9—C12	121.2 (5)	C16—C17—H17	120.00
C8—C9—C12	121.8 (4)	C18—C17—H17	120.00
C9—C10—C11	118.7 (5)	C13—C18—H18	119.00
N3—C11—C10	124.0 (5)	C17—C18—H18	119.00
O1—C13—C14	124.4 (4)	N4—C19—H19	116.00
O1—C13—C18	118.8 (4)	C14—C19—H19	116.00
C11—Cu1—O1—C13	-113.3 (4)	C11—N3—C7—C8	3.8 (8)
N1—Cu1—O1—C13	129.3 (4)	C7—N3—C11—C10	-2.4 (9)
N3—Cu1—O1—C13	17.9 (5)	Cu1—N4—C7—N3	-17.2 (5)
N4—Cu1—O1—C13	1.5 (4)	Cu1—N4—C7—C8	161.1 (4)
C11—Cu1—N1—C1	52.5 (4)	C19—N4—C7—N3	162.7 (4)
C11—Cu1—N1—C5	-123.3 (3)	C19—N4—C7—C8	-19.0 (7)
O1—Cu1—N1—C1	169.6 (4)	Cu1—N4—C19—C14	1.3 (7)
O1—Cu1—N1—C5	-6.1 (3)	C7—N4—C19—C14	-178.6 (5)
N3—Cu1—N1—C1	-43.6 (4)	N1—C1—C2—C3	-1.3 (7)
N3—Cu1—N1—C5	140.6 (3)	N2—C1—C2—C3	-179.5 (5)
N4—Cu1—N1—C1	-87.2 (4)	C1—C2—C3—C4	-0.8 (7)
N4—Cu1—N1—C5	97.0 (4)	C1—C2—C3—C6	179.6 (4)
C11—Cu1—N3—C7	104.9 (3)	C2—C3—C4—C5	1.8 (7)
O1—Cu1—N3—C7	-30.1 (4)	C6—C3—C4—C5	-178.6 (4)
N1—Cu1—N3—C7	-143.8 (3)	C3—C4—C5—N1	-0.7 (7)
N4—Cu1—N3—C7	-9.1 (3)	N3—C7—C8—C9	-2.2 (8)

C11—Cu1—N4—C7	-68.9 (3)	N4—C7—C8—C9	179.8 (5)
C11—Cu1—N4—C19	111.2 (4)	C7—C8—C9—C10	-1.1 (7)
O1—Cu1—N4—C7	177.2 (3)	C7—C8—C9—C12	177.9 (5)
O1—Cu1—N4—C19	-2.7 (4)	C8—C9—C10—C11	2.4 (8)
N1—Cu1—N4—C7	70.6 (4)	C12—C9—C10—C11	-176.6 (5)
N1—Cu1—N4—C19	-109.3 (4)	C9—C10—C11—N3	-0.7 (9)
N3—Cu1—N4—C7	9.4 (3)	O1—C13—C14—C15	178.6 (5)
N3—Cu1—N4—C19	-170.5 (4)	O1—C13—C14—C19	-3.8 (8)
Cu1—O1—C13—C14	1.3 (7)	C18—C13—C14—C15	-0.3 (7)
Cu1—O1—C13—C18	-179.9 (3)	C18—C13—C14—C19	177.3 (5)
Cu1—N1—C1—N2	4.9 (6)	O1—C13—C18—C17	-179.9 (5)
Cu1—N1—C1—C2	-173.4 (3)	C14—C13—C18—C17	-1.0 (8)
C5—N1—C1—N2	-179.4 (5)	C13—C14—C15—C16	0.6 (8)
C5—N1—C1—C2	2.4 (6)	C19—C14—C15—C16	-177.2 (5)
Cu1—N1—C5—C4	174.7 (4)	C13—C14—C19—N4	2.4 (9)
C1—N1—C5—C4	-1.4 (7)	C15—C14—C19—N4	-179.9 (5)
Cu1—N3—C7—N4	10.8 (3)	C14—C15—C16—C17	0.3 (9)
Cu1—N3—C7—C8	-167.5 (5)	C15—C16—C17—C18	-1.6 (9)
C11—N3—C7—N4	-177.9 (5)	C16—C17—C18—C13	2.0 (8)

Hydrogen-bond geometry (Å, °)

<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>
N2—H2NB...N3	0.85 (4)	2.27 (4)	3.039 (6)	150 (5)
N2—H2NA...C11 ⁱ	0.86 (4)	2.44 (4)	3.305 (5)	179 (7)

Symmetry code: (i) *x*, -*y*+1/2, *z*-1/2.