

Cai-Feng Ding,<sup>a</sup> Xue-Mei Li,<sup>a</sup>  
Mei Zhu,<sup>a</sup> Hong Xu<sup>b</sup> and  
Shu-Sheng Zhang<sup>a\*</sup><sup>a</sup>College of Chemistry and Molecular  
Engineering, Qingdao University of Science and  
Technology, 266042 Qingdao, Shandong,  
People's Republic of China, and <sup>b</sup>College of Life  
Science and Pharmaceutical Engineering,  
Nanjing University of Technology, 210093  
Nanjing, Jiangsu, People's Republic of China

Correspondence e-mail: shushzhang@126.com

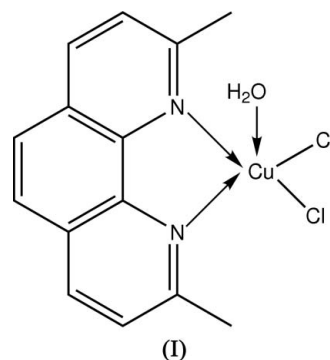
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.107  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Aquadichloro(2,9-dimethyl-1,10-phenanthroline- $\kappa^2N,N$ )copper(II)

In the title compound,  $[\text{CuCl}_2(\text{C}_{14}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$ , there are two molecules in the asymmetric unit; both Cu atoms are five-coordinate with a distorted trigonal-bipyramidal geometry. Molecules are linked into a three-dimensional network by  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds. The packing is stabilized by  $\pi-\pi$  interactions between the phenanthroline ring systems.

## Comment

In our ongoing studies of adipate-metal complexes, the title compound, (I), was obtained unexpectedly from the reaction of 2,9-dimethyl-1,10-phenanthroline and  $\text{CuCl}_2$ .



There are two molecules in the asymmetric unit; the chemically analogous bond lengths and angles of these two molecules are similar (Table 1). However, the molecules differ in the orientation of the phenanthroline ligands with respect to the Cu atoms (Fig. 1). Each  $\text{Cu}^{\text{II}}$  atom is five-coordinated by two N atoms from a 9,10-dimethylphenanthroline ligand, the O atom from a water molecule and two Cl atoms. The  $\text{CuON}_2\text{Cl}_2$  unit forms a distorted trigonal-bipyramidal geometry, with one O atom and one N atom occupying the axial positions [ $\text{O1}-\text{Cu1}-\text{N1} = 175.0$  (1) $^\circ$  and  $\text{O2}-\text{Cu2}-\text{N4} = 172.7$  (2) $^\circ$ ].

In the crystal structure, molecules are linked into a three-dimensional network by  $\text{O}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds (Table 2 and Fig. 2). The short  $\text{Cg7}\cdots\text{Cg7}^{\text{vi}}$  distance of 3.551 Å [ $\text{Cg7}$  is the centroid of the  $\text{C5}-\text{C8}/\text{C12}/\text{C13}$  ring; symmetry code: (vi)  $2-x, 2-y, -z$ ] indicates  $\pi-\pi$  stacking interactions between the phenanthroline ring systems, which contribute to the crystal packing.

## Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline (0.21 g, 1 mmol) and adipic acid (0.73 g, 0.5 mmol) in ethanol (10 ml) was added a

Received 5 January 2006  
Accepted 20 February 2006

solution of  $\text{CuCl}_2$  (0.14 g, 1 mmol) in distilled water (10 ml). The mixture was stirred and refluxed for 5 h. A hot solution was filtered into another flask containing a mixture of ethanol–methanol (1:2 v/v). Green crystals appeared over a period of a week by slow evaporation at room temperature.

#### Crystal data

$[\text{CuCl}_2(\text{C}_{14}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$   
 $M_r = 360.71$   
 Triclinic,  $P\bar{1}$   
 $a = 7.5047$  (6) Å  
 $b = 11.3643$  (9) Å  
 $c = 19.3670$  (15) Å  
 $\alpha = 100.981$  (1)°  
 $\beta = 100.913$  (1)°  
 $\gamma = 104.753$  (1)°  
 $V = 1518.0$  (2) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.578$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3160 reflections  
 $\theta = 2.4$ – $26.0$ °  
 $\mu = 1.79$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, green  
 $0.22 \times 0.12 \times 0.07$  mm

#### Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.695$ ,  $T_{\max} = 0.885$   
 8719 measured reflections

5846 independent reflections  
 4664 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 26.0$ °  
 $h = -9 \rightarrow 9$   
 $k = -9 \rightarrow 13$   
 $l = -23 \rightarrow 19$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.107$   
 $S = 1.02$   
 5846 reflections  
 377 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.7477P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>

**Table 1**  
Selected bond lengths (Å).

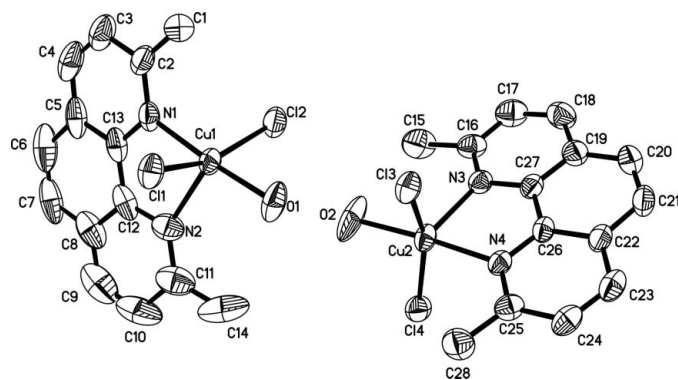
Cu1—O1	1.960 (3)	Cu2—O2	1.942 (3)
Cu1—N1	1.997 (3)	Cu2—N4	2.000 (2)
Cu1—N2	2.227 (3)	Cu2—N3	2.241 (3)
Cu1—Cl2	2.3074 (10)	Cu2—Cl4	2.3109 (10)
Cu1—Cl1	2.3144 (10)	Cu2—Cl3	2.3194 (9)

**Table 2**  
Hydrogen-bond geometry (Å, °).

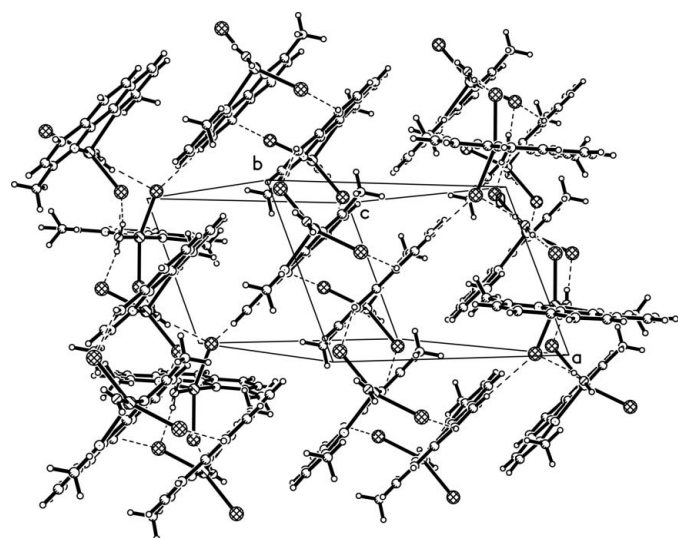
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1O1 $\cdots$ C13	0.84 (6)	2.31 (6)	3.121 (4)	164 (5)
O2—H1O2 $\cdots$ C12	0.63 (5)	2.49 (5)	3.096 (5)	163 (5)
O1—H2O1 $\cdots$ Cl4 <sup>i</sup>	0.73 (6)	2.46 (6)	3.149 (4)	159 (6)
O2—H2O2 $\cdots$ Cl1 <sup>ii</sup>	0.78 (6)	2.27 (6)	3.039 (5)	166 (5)
C4—H4A $\cdots$ Cl1 <sup>iii</sup>	0.93	2.80	3.601 (5)	145
C10—H10A $\cdots$ Cl1 <sup>iv</sup>	0.93	2.80	3.624 (6)	149
C23—H23A $\cdots$ Cl3 <sup>v</sup>	0.93	2.79	3.511 (4)	135

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

C-bound H atoms were refined using a riding model, with C—H = 0.93–0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The H atoms of the water molecules were located in a difference Fourier



**Figure 1**  
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.



**Figure 2**  
The molecular packing, showing the  $\pi$ – $\pi$  interactions. Hydrogen bonds are indicated by dashed lines.

map and refined isotropically; the resulting distances are given in Table 2.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

This project was supported by the Project of Educational Administration of Shandong Province (No. J04B12) and the Outstanding Adult–Young Scientific Research Encouraging Foundation of Shandong Province (No. 2005BS04007).

#### References

- Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.