μ-Adipato-κ⁴O,O′;O″,O‴-bis[chloro(2,9-dimethyl-1,10-phenanthroline-κ²N,N)-copper(II)] dihydrate

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In the centrosymmetric title compound, $[Cu_2(C_6H_8O_4)_2Cl_2$-$(C_{14}H_{12}N_2)_2]\cdot2H_2O$, each Cu atom is five-coordinate with a distorted tetragonal–pyramidal geometry. The molecules form stacks with short interplanar distances (3.328 and 3.371 Å) between neighbouring phenanthroline ligands, suggesting strong π–π interactions. The stacks are arranged in two types of layer, which differ in the direction of the normal to the phenanthroline ligands. The crystal structure is built up from alternating layers of these two types.

Comment

In our ongoing studies of adipate–metal complexes, the title compound, (I), was obtained. The present X-ray crystallographic analysis was undertaken in order to establish the stereochemistry of (I).

(I)
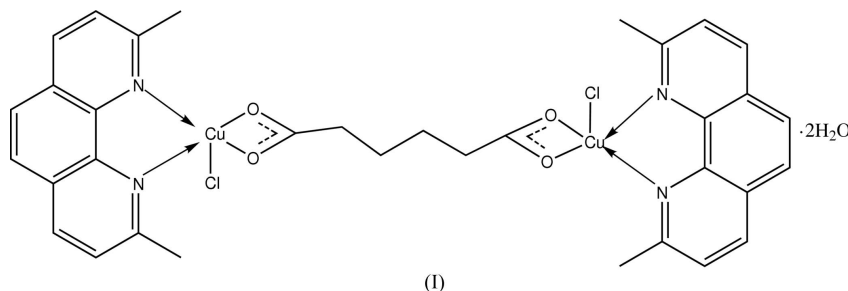
The binuclear copper complex in (I) possesses a crystallographically imposed centre of symmetry (Fig. 1). Each Cu[II] atom is five-coordinated by two N atoms from one 2,9-dimethyl-1,10-phenanthroline ligand, two O atoms from one adipate anion and one Cl atom (Table 1). This CuO_2N_2Cl coordination forms a distorted tetragonal–pyramidal geometry. The apical position is occupied by the Cl atom, with a Cu—Cl distance of 2.350 (1) Å. The N and O atoms form the square basal plane.

In the crystal structure (Fig. 2), the short interplanar distances of 3.328 and 3.371 Å between neighbouring phenanthroline ligands suggest strong π–π interactions. The distances between the centroids Cgn of rings N1/C2–C5/C12 (Cg1), N2/C8–C11/C13 (Cg2) and C5/C8/C12/C13 (Cg3) are $Cg1\cdots Cg2^i$ = 3.562 (1), $Cg1\cdots Cg3^{ii}$ = 3.685 (1) and $Cg2\cdots Cg3^i$ = 3.609 (1) Å [symmetry codes: (i) $-1-x$, $-y$, $-1-z$; (ii) $-x$, $-y$, $-1-z$]. The molecules of (I) form stacks via these π–π interactions, which are arranged in layers parallel to the ac plane. There are two types of layer, which differ in the direction of the normal to the phenanthroline ligands. The crystal structure is built up from alternating layers of these two types.
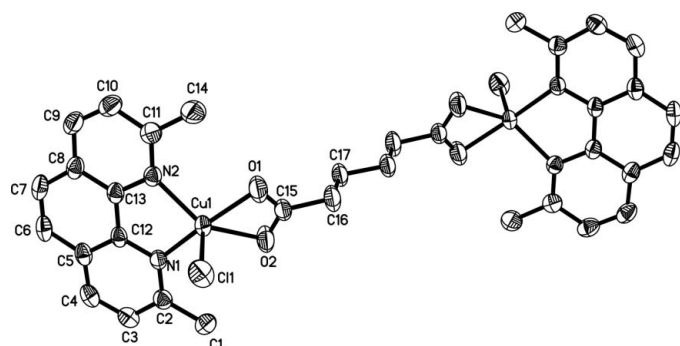
Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms and water O molecules have been omitted for clarity. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x, -y, -z)$.

Experimental

The title compound was prepared according to the literature method of Ding *et al.* (2005). Pale-green crystals of (I) appeared over a period of one week by slow evaporation of an ethanol solution at room temperature.

Crystal data

$[Cu_2(C_6H_8O_4)_2Cl_2(C_{14}H_{12}N_2)_2Cl_2]\cdot 2H_2O$	$D_x = 1.604$ Mg m^{-3}
$M_r = 794.65$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5751 reflections
$a = 8.2277$ (5) Å	$\theta = 2.7$–$26.0°$
$b = 14.9414$ (9) Å	$\mu = 1.51$ mm^{-1}
$c = 14.3046$ (7) Å	$T = 293$ (2) K
$\beta = 110.639$ (3)$°$	Block, pale green
$V = 1645.65$ (16) Å^3	$0.36 \times 0.23 \times 0.16$ mm
$Z = 2$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3224 independent reflections
ω scans	2968 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.012$
$T_{min} = 0.613$, $T_{max} = 0.795$	$\theta_{max} = 26.0°$
9115 measured reflections	$h = -10 \rightarrow 9$
	$k = -14 \rightarrow 18$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.7308P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.16$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
3224 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
217 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

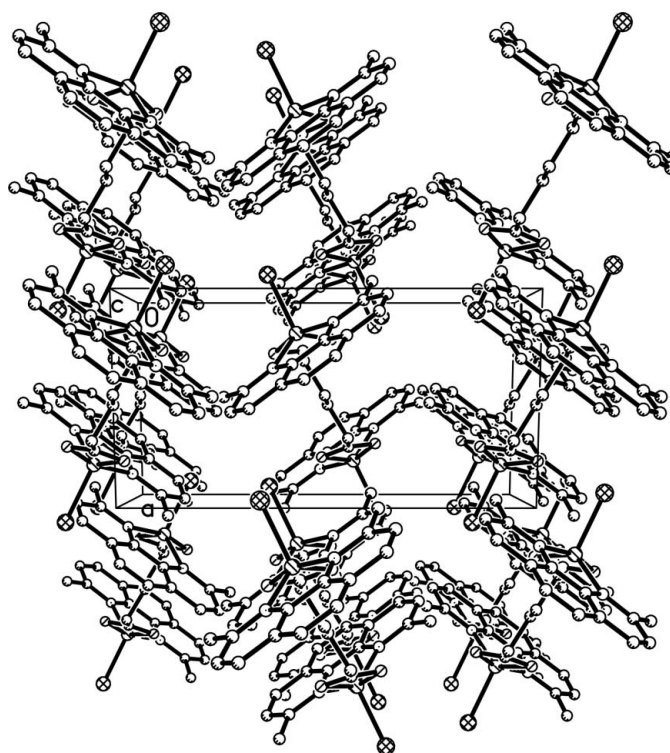|			
Cu1—O1	1.9828 (17)	Cu1—O2	2.1606 (17)
Cu1—N1	1.9966 (17)	Cu1—Cl1	2.3502 (7)
Cu1—N2	2.0685 (17)		

Figure 2
The crystal packing of (I), viewed down the *c* axis. H atoms and water molecules have been omitted for clarity.

The C-bound H atoms were geometrically positioned and refined using a riding model, with C—H bond distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2$–1.5 $U_{eq}(C)$. The H atoms of the water molecules were not located in the final difference Fourier map due to the limitations of the data.

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).

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