Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Aqua(1,10-phenanthroline)bis(trichloroacetato)-copper(II)

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Received 11 August 2005
Accepted 19 August 2005
Online 27 August 2005

In the title compound, $[Cu(C_2Cl_3O_2)_2(C_{12}H_8N_2)(H_2O)]$, the copper(II) ion is five-coordinated by four basal atoms (two N atoms from a 1,10-phenanthroline molecule and two O atoms from two trichloroacetate anions) and one axial aqua molecule, in a distorted square-pyramidal coordination geometry. Moreover, two adjacent mononuclear units are associated by intra- and intermolecular O—H···O hydrogen bonds to form a grid dimer. The hydrogen-bonding pattern could be described in graph-set terminology as $R_1^1(6)R_1^2(8)$.

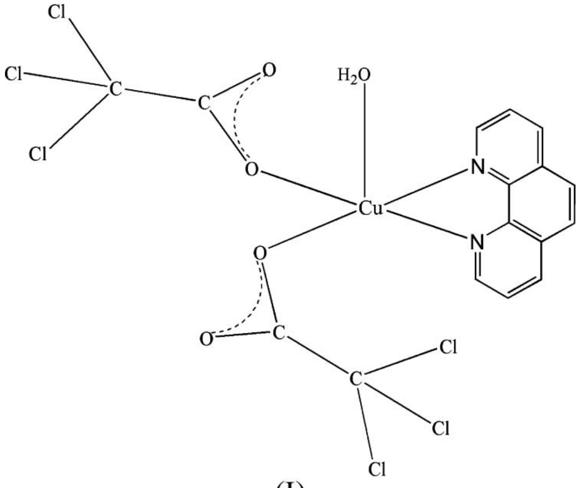
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.013 Å
R factor = 0.083
wR factor = 0.167
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Five-coordinate copper(II) complexes have geometries ranging from trigonal-bipyramidal to square-pyramidal. Energetically, the limiting trigonal-bipyramidal and square-pyramidal forms are often almost equally favorable, with a low activation barrier to interconversion. Two such copper(II) complexes, $[Cu(C_3H_3N_2)(C_{12}H_8N_2)Cl]_n$ and $[Cu(C_6H_6N_4)Cl_2]_n$ have been reported by us (Hu *et al.*, 2004, 2005). To extend this research, we report here the crystal structure of the title compound, $[Cu(C_2Cl_3O_2)_2(C_{12}H_8N_2)(H_2O)]$, (I).



(I)

In (I), each Cu ion is five-coordinated, with a distorted square-pyramidal geometry (Fig. 1 and Table 1), as determined by the observed distortion value τ (Van Albada *et al.*, 1999; Addison *et al.*, 1984) of 0.184, which is near the ideal value of τ = 0. For perfect trigonal-bipyramidal geometry, τ = 1. The basal plane is formed by atoms N1 and N2 from one 1,10-phenanthroline ligand in chelating mode, along with atoms O1 and O3 from two trichloroacetate anions with an r.m.s. deviation of 0.1406 Å. The apical site is occupied by an aqua molecule. Atom Cu1 is located 0.226 (2) Å out of the

doi:10.1107/S1600536805026644

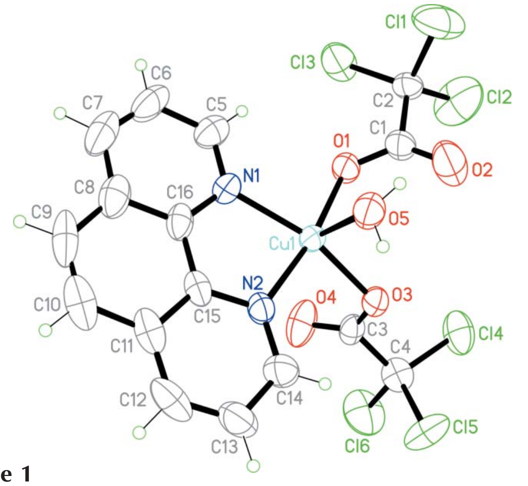


Figure 1
The mononuclear unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

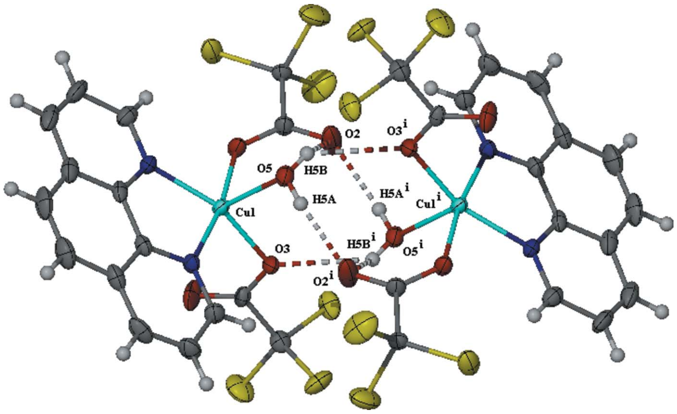


Figure 2
The grid dimer of (I) formed by O—H···O hydrogen bond interactions, which are shown as dashed lines. [Symmetry code: (i) $2 - x, 2 - y, 1 - z$.]

basal plane towards O5. Moreover, two adjacent mononuclear units are associated by intramolecular O5—H5B···O2 and intermolecular O5—H5A···O2^{i} and O5—H5B···O3^{i} [symmetry codes: (i) $2 - x, 2 - y, 1 - z$] hydrogen bonds to form a grid dimer (Fig. 2 and Table 2). The hydrogen-bonding pattern, as shown in Fig. 2, could be described in graph-set terminology (Etter, 1990; Grell *et al.*, 2000) as $R_1^1(6)R_1^2(8)$.

Experimental

The title compound was synthesized by a hydrothermal method from a mixture of trichloroacetic acid (2 mmol, 0.32 g), $CuCl_2{\cdot}2H_2O$ (1 mmol, 0.17 g) and 1,10-phenanthroline (2 mmol, 0.36 g), along with water (20 ml) in a 30 ml Teflon-lined stainless steel reactor. The solution of (I) was heated to 418 K for three days. After the reaction system had been cooled slowly to room temperature, blue prismatic crystals were collected and washed with distilled water.

Crystal data

$[Cu(C_2Cl_3O_2)_2(C_{12}H_8N_2)(H_2O)]$
$M_r = 586.51$
Monoclinic, $P2_1/c$
$a = 11.8410$ (7) Å
$b = 12.5940$ (8) Å
$c = 17.8365$ (8) Å
$\beta = 123.817$ (3)°
$V = 2209.9$ (2) Å^3
$Z = 4$

$D_x = 1.763$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3444 reflections
$\theta = 2.3$–24.2°
$\mu = 1.75$ mm^{-1}
$T = 298$ (2) K
Prism, blue
0.22 × 0.15 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.700$, $T_{max} = 0.818$
20876 measured reflections

3892 independent reflections
3535 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.0°$
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.167$
$S = 1.31$
3892 reflections
277 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 6.2996P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.943 (4)	Cu1—N1	2.027 (5)
Cu1—O3	1.968 (4)	Cu1—O5	2.243 (5)
Cu1—N2	2.002 (5)	Cu1—O4	2.844 (4)
O1—Cu1—O3	95.13 (18)	N2—Cu1—N1	81.9 (2)
O1—Cu1—N2	170.75 (19)	O1—Cu1—O5	95.14 (19)
O3—Cu1—N2	92.70 (19)	O3—Cu1—O5	96.70 (17)
O1—Cu1—N1	89.04 (19)	N2—Cu1—O5	88.83 (19)
O3—Cu1—N1	159.72 (19)	N1—Cu1—O5	102.69 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2^{i}	0.82 (2)	1.97 (3)	2.765 (7)	161 (7)
O5—H5B···O3^{i}	0.82 (2)	2.46 (5)	2.972 (6)	121 (5)
O5—H5B···O2	0.82 (2)	2.45 (6)	3.056 (9)	131 (6)

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

The aromatic H atoms were placed at calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 (2) Å and H···H = 1.39 (1) Å; their displacement parameters could not be refined and were instead similarly tied.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

We acknowledge financial support by the Zhejiang Provincial Technology Project Foundation of China (No. 2004 C32088), the Zhejiang Provincial Natural Science Foundation of China (No. 202137) and the National Natural Science Foundation of China (No. 20471043).

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