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Bis[(acetato-κO)bis(2,2′-bipyridine-$\kappa^2 N,N'$)-copper(II)] 4-carboxyphenoxyacetate hexahydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.106
Data-to-parameter ratio = 16.1

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

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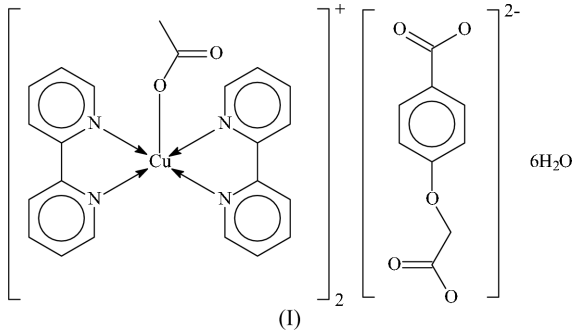
The Cu atoms in the two independent cations of the title compound, $[Cu(C_2H_3O_2)(C_{10}H_8N_2)_2]_2(C_9H_6O_5)\cdot 6H_2O$, show square-pyramidal coordination, with one N atom of a chelating heterocycle occupying the apical site. The anions interact, *via* hydrogen bonds, with the solvent water molecules to form sheets, and the cations occupy the spaces between the sheets.

Comment

We have reported previousy a small number of metal complexes of 4-carboxyphenoxyacetic acid, $HO_2CC_6H_4O$-CH_2CO_2H, *e.g.* the tetraaquamagnesium complex (Gao, Li *et al.*, 2004) and a zinc 4,4′-bipyridine complex (Gao, Huo *et al.*, 2004). These studies have been extended to the present copper 2,2′-bipridine complex, (I).



(I)

In the reaction of copper diacetate with 2,2′-bipyridine, only one acetate group is replaced, the product being the hexahydrate title salt, illustrated in Fig. 1. Selected bond distances and angles are given in Table 1. The two independent cations each have their metal atoms in a square-pyramidal geometry; there is no coordination by the 4-carboxyphenoxyacetate dianion. The dianion interacts with the solvent water molecules, *via* hydrogen bonds, to form sheets (details are given in Table 2). The two cations show non-crystallographic symmetry with respect to one another; that involving atom Cu1 is approximately related to that involving atom Cu2 by the symmetry operation $(\frac{1}{2}-x, \frac{1}{2}-y, 1-z)$.

The structural literature lists two such cations; one is a hydrate with the bis(oxalato)bis(2,2′-bipyridyl)copper-chromate anion (Costisor *et al.*, 2001) and the other is a chloride that has methanol and four water solvent molecules (Carballo *et al.*, 2003). These Cu atoms also show square-pyramidal geometry.

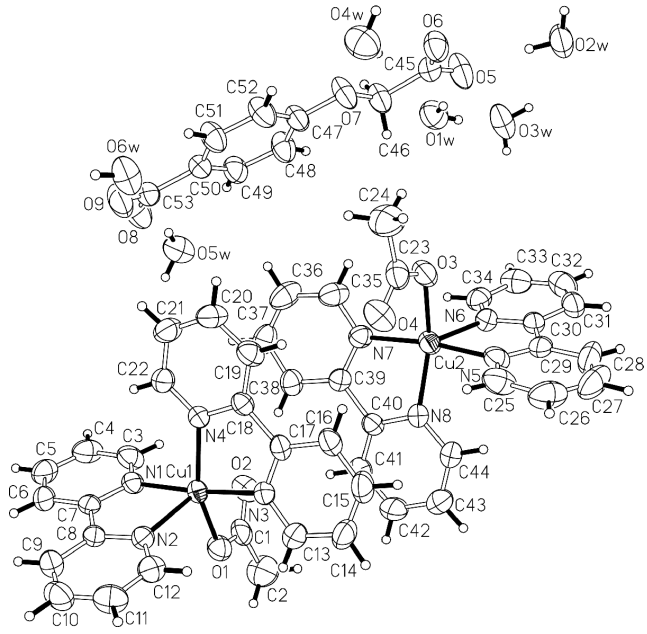


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.

Experimental

Copper diacetate monohydrate (4.00 g, 20 mmol) and 2,2′-bipyridine (2.12 g, 20 mmol) were added to an aqueous solution of 3-carboxyphenoxyacetic acid (1.96 g, 10 mmol). The solution was heated and the pH adjusted to 7, with several drops of 0.1 *M* sodium hydroxide, to give a clear solution. Blue prism-shaped crystal deposited from the solution after several days. Analysis calculated for $C_{53}H_{56}Cu_2N_8O_{15}$: C 54.31, H 4.82, N 9.56%; found: C 54.19, H 4.74, N 9.61%.

Crystal data

$[Cu(C_2H_3O_2)(C_{10}H_8N_2)_2]_2$-$(C_9H_6O_5)\cdot 6H_2O$
M_r = 1172.14
Triclinic, $P\overline{1}$
a = 14.385 (2) Å
b = 14.605 (2) Å
c = 14.655 (2) Å
α = 86.95 (3)°
β = 67.22 (3)°
γ = 70.38 (3)°
V = 2663.5 (7) Å^3
Z = 2
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24035 reflections
θ = 3.3–27.4°
μ = 0.88 mm^{-1}
T = 295 (2) K
Prism, blue
0.39 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.490, T_{max} = 0.851
25444 measured reflections
11950 independent reflections
7589 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.4°
$h = -18 \rightarrow 18$
$k = -18 \rightarrow 18$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.106
S = 0.98
11950 reflections
741 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.976 (2)	Cu2—O3	1.964 (2)
Cu1—N1	2.006 (2)	Cu2—N5	2.016 (2)
Cu1—N2	2.193 (2)	Cu2—N6	2.206 (2)
Cu1—N4	2.048 (2)	Cu2—N7	2.012 (2)
Cu1—N3	1.998 (2)	Cu2—N8	2.020 (2)
O1—Cu1—N1	92.96 (9)	O3—Cu2—N5	91.58 (9)
O1—Cu1—N2	96.28 (8)	O3—Cu2—N6	93.97 (8)
O1—Cu1—N3	91.67 (9)	O3—Cu2—N7	92.38 (9)
O1—Cu1—N4	155.77 (8)	O3—Cu2—N8	164.46 (8)
N1—Cu1—N2	78.46 (8)	N5—Cu2—N6	77.76 (9)
N1—Cu1—N3	174.85 (8)	N5—Cu2—N7	171.03 (9)
N1—Cu1—N4	94.85 (9)	N5—Cu2—N8	93.70 (9)
N2—Cu1—N3	103.30 (8)	N6—Cu2—N7	109.96 (8)
N2—Cu1—N4	107.74 (8)	N6—Cu2—N8	101.42 (9)
N3—Cu1—N4	80.00 (9)	N7—Cu2—N8	80.48 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w2···O5	0.86 (1)	1.90 (1)	2.748 (3)	168 (4)
O1w—H1w1···O3w	0.84 (1)	2.08 (1)	2.898 (4)	162 (3)
O2w—H2w1···O5	0.85 (1)	1.91 (1)	2.762 (3)	174 (4)
O2w—H2w2···O6^{i}	0.85 (1)	2.07 (2)	2.855 (3)	154 (4)
O3w—H3w1···O9^{ii}	0.84 (1)	2.00 (1)	2.843 (3)	178 (4)
O3w—H3w2···O3w^{iii}	0.86 (1)	2.21 (3)	2.959 (7)	146 (5)
O4w—H4w1···O6	0.84 (1)	2.30 (2)	3.081 (3)	155 (3)
O4w—H4w2···O6w^{iv}	0.85 (1)	2.02 (1)	2.858 (4)	168 (4)
O5w—H5w1···O8	0.86 (1)	1.92 (2)	2.757 (4)	165 (4)
O5w—H5w2···O1w^{v}	0.85 (1)	1.95 (1)	2.799 (3)	175 (4)
O6w—H6w1···O9	0.85 (1)	1.91 (1)	2.754 (4)	171 (4)
O6w—H6w2···O2w^{vi}	0.85 (1)	1.97 (1)	2.794 (4)	163 (3)

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

The water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å; U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were placed in calculated positions and treated as riding atoms [aromatic C—H = 0.93 Å and aliphatic C—H = 0.96 Å; U_{iso}(H) = 1.2U_{eq}(C)].

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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