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(Acetylenedicarboxylato)diaqua(1,10-phenanthroline)copper(II) dihydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.077
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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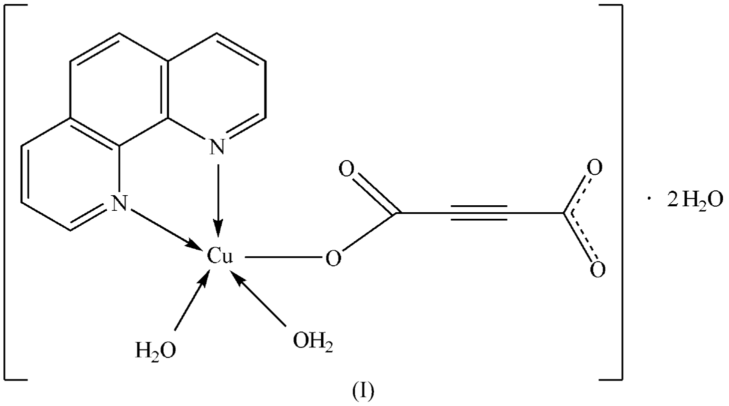
In the title complex, $[Cu(C_4O_4)(C_{12}H_8N_2)(H_2O)_2]\cdot 2H_2O$, the Cu^{II} centre exhibits a slightly distorted square-pyramidal coordination geometry, defined by two N atoms from a 1,10-phenanthroline (phen) molecule, one O atom from an acetylenedicarboxylate dianion (ace^{2-}), and two O atoms from two coordinated water molecules.

Comment

The construction of coordination polymers and netwoks by the self-assembly of polycarboxylic acids and metal ions is a rapidly growing area of reaseach (Evans & Lin, 2002). We are interested in the solid-state coordination chemistry of acetylenedicarboxylic acid, which is deemed to be a good candidate for the fabrication of versatile complexes (Pantenburg & Ruschewitz, 2002; Ruschewitz & Pantenburg, 2002). In most cases, the complete deprotonatation of the carboxylic acid groups may lead to the formation of one-, two- or three-dimensional structures in the reaction process (Stein & Ruschewitz, 2005; Wang *et al.*, 2006*a*,*b*), but there are no reports to date on this type of mononuclear complex. Recently, we isolated a new complex, $[Cu(C_{12}H_8N_2)(C_4O_4)(H_2O)_2]\cdot 2H_2O$, (I) and its structure is described here.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The Cu^{II} atom is coordinated by one O atom from one ace^{2-} ligand, two N atoms from a phen ligand and two O atoms from two coordinated water molecules, forming a slightly distorted square-pyramidal configuration, in which the apical site is occupied by atom O2*W*. The C16—O4 and C16—O3 distances are nearly identical (Table 1), suggesting delocalization of electrons. The distance between Cu1 and O1 [2.886 (1) Å] is long, indicating no bonding.

A supramolecular network is constructed *via* hydrogen-bonding interactions (Table 2).

Experimental

The title complex was prepared by the addition of stoichiometric amounts of $Cu(OAc)_2 \cdot H_2O$ (0.400 g, 2 mmol), NaOH (0.160 g, 4 mmol) and 1,10-phenanthroline (0.398 g, 2 mmol) to a hot ethanol–water (1:1 *v*/*v*) solution (20 ml) of acetylenedicarboxylic acid (0.288 g, 2 mmol), with subsequent fltration. Blue crystals of (I) were obtained from the filtered solution at room temperature over a period of 5 d. Analysis, calculated for $C_{16}H_{16}CuN_2O_8$: C 44.92, H 3.77, N 6.55%; found: C 44.83, H 3.71, N 6.44%.

Crystal data

$[Cu(C_4O_4)(C_{12}H_8N_2)(H_2O)_2] \cdot 2H_2O$
$M_r = 427.85$
Monoclinic, $P2_1/n$
$a = 9.1304\ (18)$ Å
$b = 17.414\ (4)$ Å
$c = 10.964\ (2)$ Å
$\beta = 97.74\ (3)^\circ$
$V = 1727.3\ (6)$ Å^3
$Z = 4$
$D_x = 1.645$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.31$ mm^{-1}
$T = 295\ (2)$ K
Block, blue
0.35 × 0.25 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.656$, $T_{max} = 0.827$
16607 measured reflections
3939 independent reflections
3470 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.4^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.077$
$S = 1.06$
3939 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.8958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1*W*	1.9494 (15)	Cu1—N2	2.0186 (16)
Cu1—O2	1.9499 (14)	Cu1—O2*W*	2.2024 (15)
Cu1—N1	2.0094 (16)		
O1*W*—Cu1—O2	88.96 (7)	N1—Cu1—N2	82.09 (7)
O1*W*—Cu1—N1	170.78 (7)	O1*W*—Cu1—O2*W*	93.46 (7)
O2—Cu1—N1	95.39 (7)	O2—Cu1—O2*W*	95.23 (6)
O1*W*—Cu1—N2	92.13 (7)	N1—Cu1—O2*W*	94.23 (7)
O2—Cu1—N2	169.25 (6)	N2—Cu1—O2*W*	95.38 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*2···O4*W*	0.85	1.79	2.634 (2)	170
O1*W*—H1*W*1···O4^{i}	0.85	1.97	2.809 (2)	171
O2*W*—H2*W*1···O3^{ii}	0.85	2.26	2.832 (2)	125
O2*W*—H2*W*2···O4^{iii}	0.85	2.08	2.934 (2)	178
O3*W*—H3*W*1···O1^{ii}	0.85	2.07	2.914 (3)	176
O3*W*—H3*W*2···O1^{iv}	0.85	2.04	2.891 (3)	176
O4*W*—H4*W*1···O3*W*	0.85	1.89	2.726 (3)	169
O4*W*—H4*W*2···O3^{iii}	0.85	1.91	2.752 (2)	169

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x, y, z - 1$; (iv) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

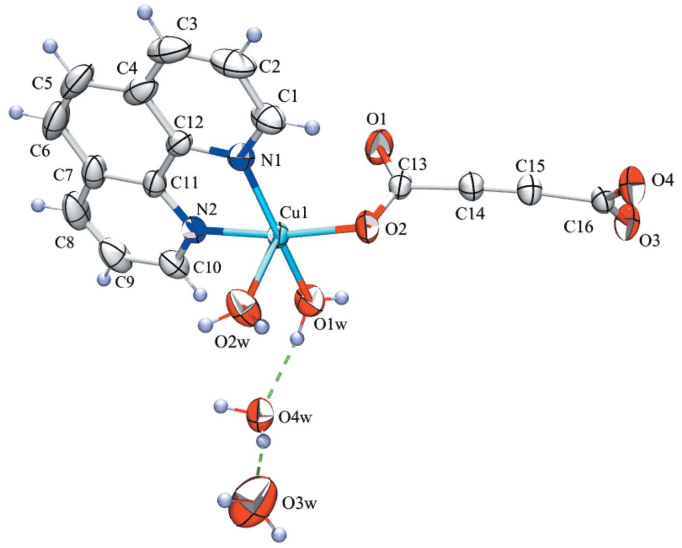


Figure 1
The molecular structure of complex (I), with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

Water H atoms were located in a difference map and refined as riding, with O—H = 0.85 Å and with $U_{iso}(H) = 1.5U_{eq}(O)$. All other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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