Crystal structure of *catena*-adipato-*O*,*O'*-diaquacopper(II), $Cu(C_6H_8O_4)(H_2O)_2$

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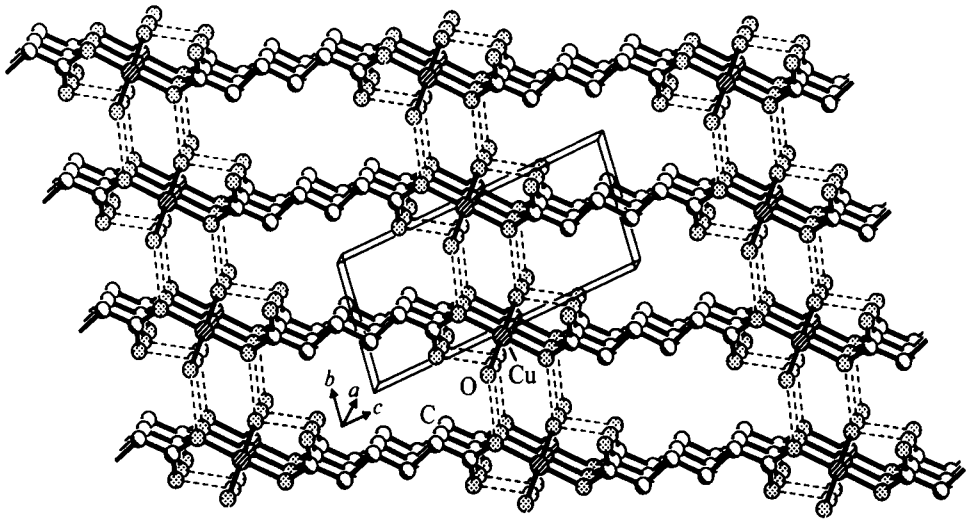

Abstract

$C_6H_{12}CuO_6$, triclinic, $P\bar{1}$ (No. 2), a = 3.861(1) Å, b = 4.928(1) Å, c = 11.326(2) Å, α = 84.34(2)°, β = 87.08(1)°, γ = 83.45(2)°, V = 212.9 Å^3, Z = 1, $R_{gt}(F)$ = 0.040, $wR_{ref}(F^2)$ = 0.104, T = 293 K.

Source of material

The title compound was synthesized by the reaction of 0.50 g (3.42 mmol) adipic acid with an excess of freshly prepared $CuCO_3$ in 50 ml doubly-destilled water, followed by removing the unreacted $CuCO_3$. Blue crystals grew from the filtrate at room temperature by slow evaporation for several weeks.

Discussion

In the crystal structure, each Cu atom is square-planarly coordinated by four O atoms from two bis-monodentate adipate ligands and two water molecules to form a *trans* configuration with d(Cu—O) = 1.930 Å (2×), 1.969 Å (2×). The Cu atom is exactly located in the least-squares plane defined by the four coordinating O atoms. Through the carboxyl O atoms on both ends, the adipate $(C_6H_8O_4)^{2-}$ ligands bridge the Cu atoms to form 1D chains $^1_\infty[Cu(C_6H_8O_4)_{2/2}(H_2O)_2]$, which propagate parallel to [0$\bar{1}$1] and are held together by interchain hydrogen bonds between water and carboxyl oxygen atoms with d(O···O) = 2.630 Å and 2.688 Å and ∠O–H···O = 154° and 169°.The adipate $(C_6H_8O_4)^{2-}$ ligands are centered at 1e positions and their bridging fashion is similar to that observed in the Co adipate reported previously [1]. All backbone C atoms are nearly coplanar and the dihedral angle between the carboxyl plane and the C backbone plane is 19.9°. The terminal C—C bonds of 1.510 Å are significantly shorter than the rests averaged at 1.523 Å and the terminal ∠C–C–C angles of 113.9° are slightly larger than the rests of 111.8°. The C—O bond length of 1.297 Å to the coordinating O atom is substantially larger than that of 1.235 Å to the non-coordinating one. The closest Cu···Cu distance of 3.861Å does not indicate interaction between the Cu atoms.

Table 1. Data collection and handling.

Crystal:	blue block, size 0.089 × 0.178 × 0.222 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	25.61 cm^{-1}
Diffractometer, scan mode:	Bruker P4, θ/2θ
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1413, 982
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 966
$N(param)_{refined}$:	62
Programs:	SHELXS-97 [2], SHELXL-97 [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	2*i*	0.3925	–0.6305	0.8100	0.028
H(2B)	2*i*	0.7504	–0.5296	0.8100	0.037
H(3A)	2*i*	0.5704	–0.2185	0.9632	0.028
H(3B)	2*i*	0.198	–0.3234	0.9689	0.027
HA(O3)	2*i*	0.2387	–0.3626	0.4156	0.050
HB(O3)	2*i*	0.1217	–0.1382	0.3597	0.050

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	1*f*	1/2	0	1/2	0.0431(3)	0.0153(3)	0.0119(3)	0.0032(2)	0.0005(2)	0.0016(2)
C(1)	2*i*	0.4047(6)	-0.2584(5)	0.7300(2)	0.029(1)	0.020(1)	0.017(1)	0.0006(8)	-0.0035(8)	0.0018(9)
C(2)	2*i*	0.5169(6)	-0.4766(5)	0.8279(2)	0.028(1)	0.022(1)	0.016(1)	0.0055(8)	0.0001(8)	0.0025(9)
C(3)	2*i*	0.4477(6)	-0.3847(5)	0.9523(2)	0.027(1)	0.024(1)	0.014(1)	0.0036(9)	-0.0001(8)	0.0023(9)
O(1)	2*i*	0.5481(6)	-0.2942(4)	0.6258(2)	0.049(1)	0.0182(8)	0.0152(9)	0.0032(7)	0.0008(7)	0.0021(7)
O(2)	2*i*	0.1904(5)	-0.0608(4)	0.7502(2)	0.039(1)	0.028(1)	0.024(1)	0.0117(8)	-0.0049(8)	0.0016(8)
O(3)	2*i*	0.1752(5)	-0.2022(4)	0.4238(2)	0.044(1)	0.0182(8)	0.0197(9)	0.0058(7)	-0.0029(7)	-0.0009(7)

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