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Key indicators

Single-crystal X-ray study
 T = 292 K
 Mean $\sigma(C-C) = 0.004 \text{ \AA}$
 R factor = 0.031
 wR factor = 0.090
 Data-to-parameter ratio = 15.4

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

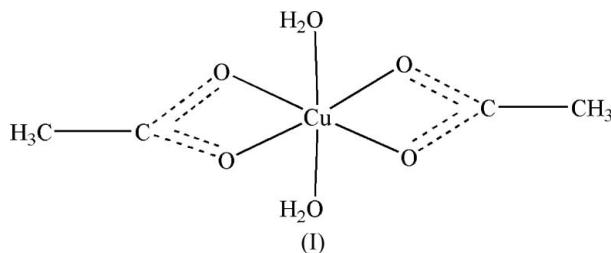
Bis(acetato- κ^2O,O')diaquacopper(II)

A new monomeric copper acetate complex, $[\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$, was obtained unexpectedly by the reaction of $\text{Cu}_2(\text{CO}_3)_2(\text{OH})_2 \cdot x\text{H}_2\text{O}$, acetonitrile, ammonia and water under hydrothermal conditions. The structure contains a discrete centrosymmetric diacetatodiaquacopper(II) complex and the Cu^{II} atom is coordinated by four O atoms from two acetate anions and two water molecules, giving a distorted octahedral geometry.

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Comment

Dimeric copper acetate monohydrate tetra- μ -acetatodiaquacopper(II) has been reported (van Niekerk & Schoening, 1953; de Meester *et al.*, 1973). We obtained a new monomeric copper acetate complex, (I), by hydrothermal reaction of $\text{Cu}_2(\text{CO}_3)_2(\text{OH})_2 \cdot x\text{H}_2\text{O}$, acetonitrile, ammonia and H_2O . Under such reaction conditions, acetonitrile could be hydrolysed to form the acetate anion, which is coordinated to the Cu atom.



The Cu^{II} atom, lying on a centre of symmetry, is coordinated by four acetate O atoms of $[\text{Cu1}-\text{O2} = 2.0051(17) \text{ \AA}$ and $\text{Cu1}-\text{O3} = 2.682(2) \text{ \AA}]$, and two water molecules $[\text{Cu1}-\text{O1} = 1.978(3) \text{ \AA}]$, giving an elongated octahedral coordination geometry (Fig. 1). This is a typical instance of the Jahn–Teller

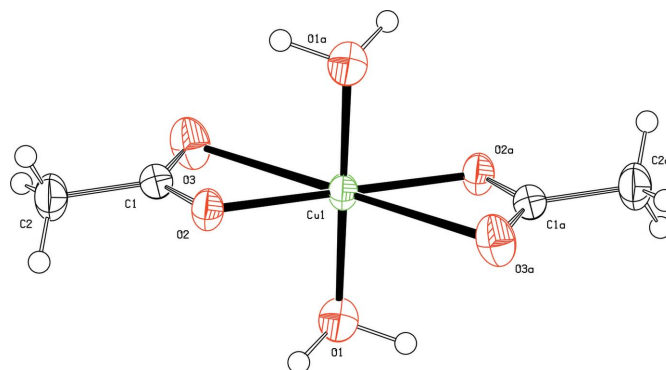


Figure 1
 The molecular structure of (I), showing labelling of the non-H atoms and 50% probability ellipsoids [symmetry code: (a) $1 - x, -y, 2 - z$].

effect. The O3—C1 distance [1.237 (3) Å] is significantly shorter than the O2—C1 distance [1.278 (3) Å], suggesting that the carboxylate group is not a completely delocalized system. The molecules are firmly linked by hydrogen bonds to form a three-dimensional network (Fig. 2).

Experimental

A mixture of $\text{Cu}_2(\text{CO}_3)_2(\text{OH})_2 \cdot x\text{H}_2\text{O}$ (0.5 g), acetonitrile (5 ml), ammonia (25%, 5 ml) and H_2O (5 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 453 K for 72 h. Blue block-shaped crystals of the title complex were obtained.

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{H}_2\text{O})_2]$	$Z = 2$
$M_r = 217.66$	$D_x = 1.803 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.4731 (7) \text{ \AA}$	$\mu = 2.71 \text{ mm}^{-1}$
$b = 10.1990 (13) \text{ \AA}$	$T = 292 (2) \text{ K}$
$c = 7.5187 (10) \text{ \AA}$	Block, blue
$\beta = 107.230 (2)^\circ$	$0.30 \times 0.20 \times 0.16 \text{ mm}$
$V = 400.86 (9) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	2290 measured reflections
φ and ω scans	907 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	825 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.482$, $T_{\max} = 0.648$	$R_{\text{int}} = 0.016$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.2477P]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
907 reflections	$\Delta\rho_{\text{min}} = -0.78 \text{ e \AA}^{-3}$
59 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1A \cdots O3 ⁱ	1.01 (3)	2.08 (3)	3.015 (3)	154 (3)
O1—H1B \cdots O2 ⁱⁱ	0.99 (4)	2.13 (4)	3.108 (3)	168 (3)

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

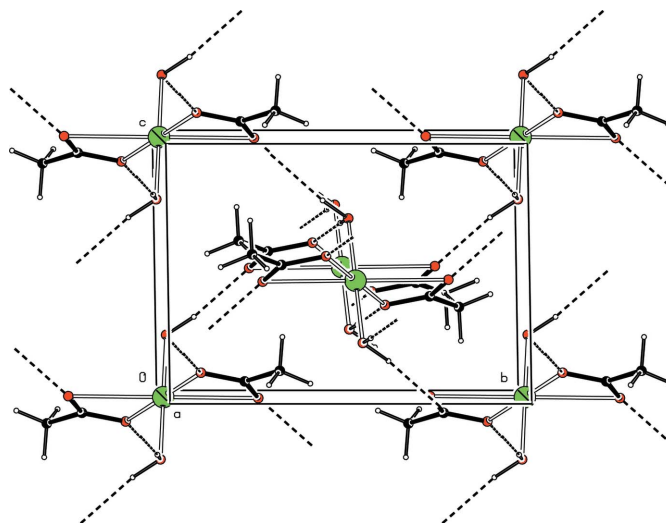


Figure 2

A packing diagram of (I), viewed along the a axis. Intermolecular O—H \cdots O hydrogen bonds are indicated by dashed lines.

Methyl H atoms were placed in geometrically idealized positions (C—H = 0.96 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. Water H atoms were located in a difference map and their positional parameters were refined, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 2000); software used to prepare material for publication: SHELXTL.

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