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catena-Poly[[aqua(diformato-κO)copper(II)]-μ-1,4-diazabicyclo[2.2.2]octane-κ^2N:N']

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Key indicators

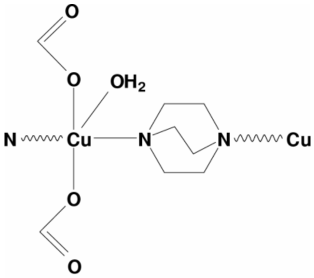
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.062
Data-to-parameter ratio = 10.9

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

The title compound, $[Cu(CHO_2)_2(C_6H_{12}N_2)(H_2O)]_n$, forms a polymeric chain, $[Cu(HCOO)_2(dabco)(H_2O)]_\infty$ (dabco is 1,4-diazabicyclo[2.2.2]octane). Both formate ligands are O-monodentate anions and dabco acts as a bridging ligand, creating a linear polymeric arrangement interconnected by $O_{water}—H\cdots O_{carboxy}$ hydrogen bonds. The deformed square-pyramidal Cu^{II} coordination comprises two N and two O atoms as the base, and a water molecule in the apical position. The point symmetry of the Cu^{II} polyhedron and the dabco ligand is *mm*, and the formate anions lie on the mirror planes $\frac{1}{4}$, *y*, *z* and $\frac{3}{4}$, *y*, *z*.

Comment

So far, Cu^{II}–dabco coordination compounds has not been intensively investigated. Only one mononuclear structure (Karan *et al.*, 1999), two dinuclear structures (Durley *et al.*, 1980; Maverick *et al.*, 1986) and one polymeric structure (Rao *et al.*, 1983) of Cu^{II} compounds containing the dabco ligand have been reported. The present paper reports the first example of the coordination of the dabco ligand in a basal position of a square-pyramidal Cu^{II} polyhedron. The structure of the title complex, (I), is polymeric, with $[Cu(HCOO)_2(dabco)(H_2O)]_\infty$ chains running along the *a* axis. In Fig. 1, the labelled atoms indicate the independent fragment of the chain.



(I)

The chain consists of pentacoordinated Cu^{II} ions in a distorted square-pyramidal (SQP) geometry, with two Cu—N bonds of 2.093 (2) Å and two Cu—O(formate) bonds of 1.962 (2) Å in the basal plane. The apical position is occupied by the water molecule [Cu—OH$_2$ = 2.238 (2) Å]. The Cu atom is displaced from the basal plane by 0.124 (1) Å towards atom O1. The point symmetry of the Cu^{II} polyhedron and the dabco ligand is *mm*, and the formate anions lie on the mirror planes $\frac{1}{4}$, *y*, *z* and $\frac{3}{4}$, *y*, *z*.

The observed SQP coordination is distinctly deformed in the direction of trigonal-bipyramidal (TBP) coordination, with

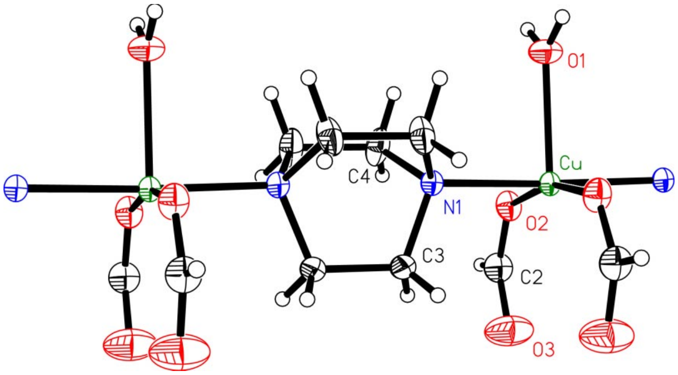


Figure 1
A fragment of the polymeric structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 40% probability level.

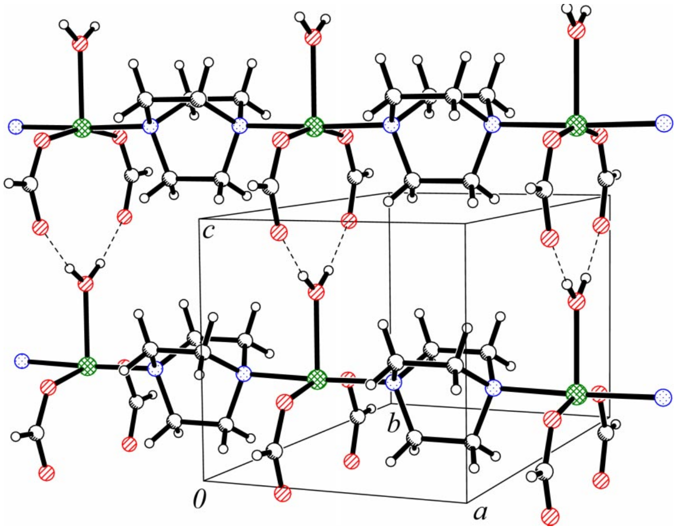


Figure 2
Perspective view of the crystal packing in the unit cell, showing the linkage of the polymeric chains by hydrogen bonding as dashed lines.

the trigonality parameter $\tau = 0.24$ [τ is defined by Addison *et al.* (1984)]; for the regular SQP structure, the trigonality parameter is 0 and for TBP distortion it increases to 1.

The formate group acts as a monodentate ligand, the distance between the Cu^{II} ion and uncoordinated atom O3 being 3.287 (3) Å. Such behaviour may be caused by the participation of this atom in a strong hydrogen bond with the water molecule. These interchain interactions, running along the *c* axis, are shown in Fig. 2. This strong hydrogen bond does not cause a delocalization of the π bond in the carboxyl group as the C2—O2 and C2—O3 bonds are distinctly different [1.257 (3) and 1.214 (4) Å, respectively].

The intrachain Cu⋯Cu distance of 6.808 (1) Å is longer than the shortest interchain Cu⋯Cu distance of 6.422 (2) Å along the *c* axis. Other short interchain Cu⋯Cu distances of 7.246 (2) and 8.157 (2) Å are between the two Cu^{II} ions related by the 2_1 screw axis, and with no spacer between them.

Experimental

The title complex was prepared by dissolving cupric formate [$Cu(HCOO)_2\cdot2H_2O$, 2 mmol] in 50 ml of water with dabco ($C_6H_{12}N_2$, 2 mmol). After heating to boiling, a few drops of formic acid were added to clear the solution. The solution was filtered and allowed to cool. After several days, turquoise crystals were obtained.

Crystal data

$[Cu(CHO_2)_2(C_6H_{12}N_2)(H_2O)]$
$M_r = 283.77$
Orthorhombic, *Pmmn*
$a = 6.8084$ (13) Å
$b = 12.071$ (2) Å
$c = 6.4224$ (15) Å
$V = 527.80$ (19) Å^3
$Z = 2$
$D_x = 1.786$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 38 reflections
$\theta = 5$–18°
$\mu = 2.08$ mm^{-1}
$T = 293$ K
Prism, turquoise
0.30 × 0.20 × 0.20 mm

Data collection

Siemens *P*3 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.557$, $T_{max} = 0.661$
719 measured reflections
719 independent reflections
710 reflections with $I > 2\sigma(I)$
$\theta_{max} = 28.0°$
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 15$
$l = 0 \rightarrow 8$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.062$
$S = 1.23$
719 reflections
66 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.21P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	2.238 (2)	O2—C2	1.257 (3)
Cu—O2	1.962 (2)	O3—C2	1.214 (4)
Cu—N1	2.093 (2)		
O1—Cu—O2	98.42 (6)	O2—Cu—O2^i	163.16 (11)
O1—Cu—N1	88.90 (5)	N1—Cu—N1^i	177.81 (9)
O2—Cu—N1	90.16 (1)		

Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, z$.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1⋯O3^{ii}	0.94 (4)	1.77 (4)	2.699 (3)	170 (4)

Symmetry code: (ii) $\frac{1}{2}-x, \frac{1}{2}-y, 1+z$.

All H atoms were located from a difference synthesis and refined isotropically. The C—H distances range from 0.92 (3) to 1.00 (4) Å and the O—H distance refined to 0.94 (4) Å.

Data collection: *P*3 (Siemens, 1993); cell refinement: *P*3; data reduction: *XDISK* in *SHELXTL/PC* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC*; software used to prepare material for publication: *PLATON* (Spek, 1990).

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