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Bis(3-carboxypropanaminium) tetrachlorocuprate(II)

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The crystal structure of the title compound, $(C_3H_{10}NO_2)_2$-$[CuCl_4]$, consists of parallel two-dimensional perovskite-type layers of corner-sharing $CuCl_6$ octahedra which are bonded together by 4-aminobutyric acid chains nearly perpendicular to the layers. The Cu atoms lie on crystallographic centers of symmetry. The layers are held together by hydrogen bonds between the 4-aminobutyric acid molecules, which are also hydrogen-bonded to $CuCl_4$ layers.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.135
Data-to-parameter ratio = 21.4

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

Comment

Copper(II) halides exhibit a wide variety of stereochemical complexity (Willett, 1991; Weise & Willett, 1993). Observed geometries include four-, five- and six-coordinate species. The flexibility of the Cu^{II} coordination sphere and the non-stereospecific nature of the halide anions, modulated by the size and hydrogen-bonding properties of the cation, allow this large span of observed geometries (Bond *et al.*, 1990).

The perovskite-layer copper chlorides with the general formulae $(C_nH_{2n+1}NH_3)_2CuCl_4$ and $NH_3(CH_2)_nNH_3CuCl_4$ have attracted a great deal of attention due to their magnetic properties and interesting structural phase transitions. However, in our recent investigations, 4-aminobutyric acid was used instead as a template and a perovskite-layer copper chloride was also obtained. We report here the synthesis and crystal structure of the title compound $[NH_3(CH_2)_3COOH]_2$-$[CuCl_4]$, (I).

$$2H_3\overset{+}{N}{-}CH_2{-}CH_2{-}CH_2{-}COOH\ \cdot\left[CuCl_4\right]^{2-}$$

X-ray crystallography reveals that the structure of (I) consists of parallel two-dimensional perovskite-type $[CuCl_4]^{2-}$ layers interleaved by layers of protonated 4-aminobutyric acid cations (Fig. 1). This perovskite-type layer consists of corner-sharing octahedra in the *bc* plane (Fig. 2). The $[CuCl_4]^{2-}$ ion is nearly square, with an in-plane Cu—Cl1 bond length of 2.289 (1) Å, an out-of-plane Cu—Cl2 bond length of 2.281 (1) Å and a Cl1—Cu—Cl2 angle of 89.95 (3)° (Table 1). The distance of Cu to the in-plane Cl1 atom of the next $[CuCl_4]^{2-}$ ion is 2.956 (1) Å and is significantly longer than the distances of 2.289 (1) and 2.281 (1) Å (4 + 2 coordination of Cu) due to the Jahn–Teller effect. Bond distance and angles are consistent with those of $CuCl_6$ octahedra in similar compounds (Tichý *et al.*, 1978).

As shown in Fig. 1, in the *bc* plane the Cu atoms and Cl1 atoms form a puckered plane and the Cu—Cl2 bond is nearly perpendicular to this plane. In the *bc* plane, the $CuCl_6$ octahedra are rotated alternately clockwise and anticlockwise around the *c* axis. The organic chains are arranged along the *a*

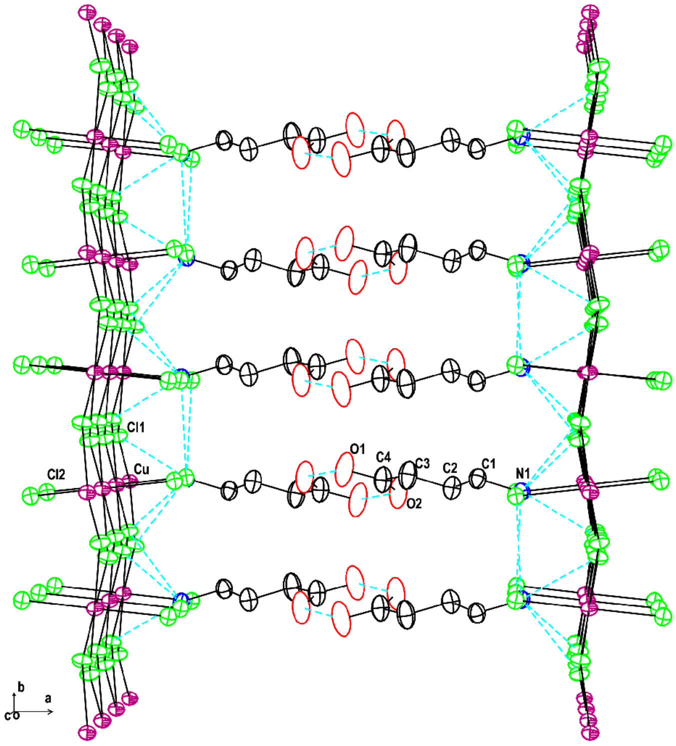

Figure 1
The crystal structure of (I), viewed along the *c* axis, with displacement ellipsoids drawn at the 30% probability level and intermolecular hydrogen bonds shown as dashed lines. H atoms have been omitted.

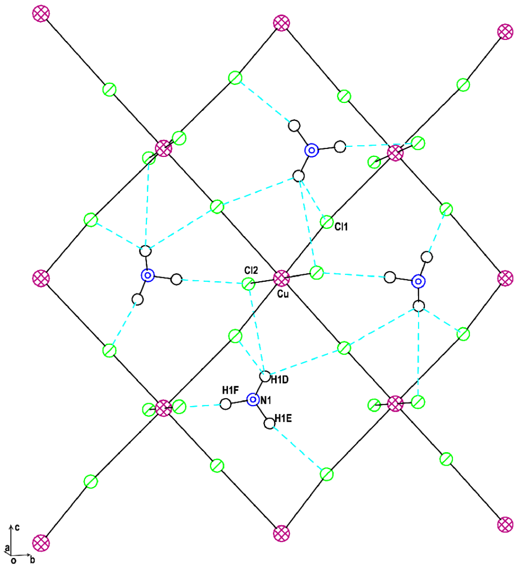

Figure 2
The crystal structure of (I), with intermolecular hydrogen bonds shown as dashed lines, viewed nearly along the *a* axis. For clarity, C, O and other H atoms have been omitted.

axis between the layers. NH_3 groups at one end of the organic chains fit into cavities of the $CuCl_4$ layer (Fig. 1) and N—H⋯Cl hydrogen bonds bind the organic chains (Fig. 2), while COOH groups at the other end of the organic chains are connected to each other by hydrogen bonds (Table 2). The structure of (I) is similar to the K_2NiF_4 structure, with Cu replacing Ni and the organic cation replacing K.

Experimental

A solution of 4-aminobutyric acid (0.206 g, 2 mmol) in 4 *M* HCl (5 ml) was added slowly to a solution of $CuCl_2{\cdot}2H_2O$ (0.171 g, 1 mmol) in 4 *M* HCl (5 ml). The reaction mixture was stirred for 1 h at room temperate and the resulting solid filtered off. The filtrate was then evaporated to give metallic yellow-coloured crystals.

Crystal data

$(C_4H_{10}NO_2)_2[CuCl_4]$
$M_r = 413.60$
Monoclinic, $P2_1/c$
$a = 15.196$ (2) Å
$b = 7.2371$ (10) Å
$c = 7.5015$ (10) Å
$\beta = 91.476$ (7)°
$V = 824.7$ (2) Å^3
$Z = 2$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 50 reflections
$\theta = 3.1$–27.5°
$\mu = 1.98$ mm^{-1}
$T = 293$ (2) K
Platelet, metallic yellow
0.22 × 0.16 × 0.06 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)
$T_{\min} = 0.691$, $T_{\max} = 0.888$
5982 measured reflections
1884 independent reflections
1646 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 27.5°$
$h = -19 \rightarrow 19$
$k = -9 \rightarrow 6$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.135$
$S = 0.97$
1884 reflections
88 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.67$ e Å^{-3}
$\Delta\rho_{\min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—Cl2	2.2806 (9)	Cu—Cl1$^{\rm i}$	2.9564 (8)
Cu—Cl1	2.2891 (7)		
Cl2—Cu—Cl1	89.96 (3)	Cl1—Cu—Cl1$^{\rm ii}$	88.327 (12)
Cl2—Cu—Cl1$^{\rm ii}$	94.15 (3)		

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

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*D*⋯Cl1$^{\rm iii}$	0.89	2.78	3.389 (3)	126
N1—H1*D*⋯Cl1$^{\rm iv}$	0.89	2.57	3.284 (3)	138
N1—H1*E*⋯Cl1	0.89	2.42	3.283 (3)	162
N1—H1*D*⋯Cl2$^{\rm v}$	0.89	2.87	3.501 (4)	129
N1—H1*F*⋯Cl2$^{\rm vi}$	0.89	2.35	3.236 (3)	172
O1—H1*C*⋯O2$^{\rm vii}$	0.82	1.79	2.613 (5)	177

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

The structure was solved by direct methods and subsequent difference Fourier synthesis. The H atoms were positioned geometrically, assigned isotropic displacement parameters and allowed to ride on their respective parent C, N and O atoms.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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