

Bis(dimethylammonium) bis(pyridine-2,5-dicarboxylato)copper(II)

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Key indicators

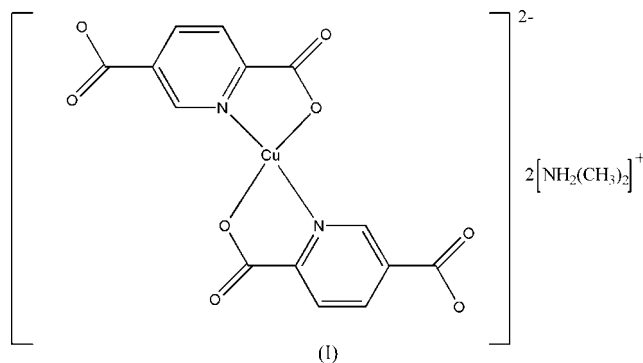
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.037
 wR factor = 0.092
Data-to-parameter ratio = 11.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $(\text{C}_2\text{H}_8\text{N})_2[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)_2]$, the Cu^{II} atom lies on an inversion centre and is coordinated in a slightly deformed square-planar geometry by two N and two O atoms from pyridine-2,5-dicarboxylate ligands. The complex anions are linked *via* weak coordination of an O atom of the 2-carboxylate group to the Cu atom of a neighbouring complex, forming chains along the a axis. There are $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds between dimethylammonium cations and the 5-carboxylate group of the ligand.

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Comment

The development of supramolecular synthons is an important aspect of crystal engineering as it generates new structures with novel architectures and topologies which, in turn, lead to new materials and properties (Zhang & Chen, 2005). The concept of preparing compounds built from metal ions and organic acids has received considerable attention in the planned assembly of supramolecular architectures (Che *et al.*, 2006). Recently, aromatic di- or poly(carboxylic acids) have been extensively investigated in the areas of solid-state and materials science (Ma *et al.*, 2003). For instance, pyridine-2,5-dicarboxylic acid (H_2pdc) has been employed in the preparation of metal-based functional solids to produce interesting structures (Tian *et al.*, 2005). In this paper, we report the crystal structure of the title compound, (I), which was prepared by a solvothermal synthesis at about 433 K. The compound, once formed, is air-stable and insoluble in most solvents. The dimethylammonium ion in (I) is believed to be the result of the decomposition of *N,N*-dimethylformamide under solvothermal conditions. This phenomenon has been commonly observed in the literature (Mahon *et al.*, 2005).



In compound (I), the Cu^{II} atom lies on an inversion centre, and is coordinated in a slightly deformed square-planar geometry by the O and N atoms from two pdc^{2-} ligands, if the

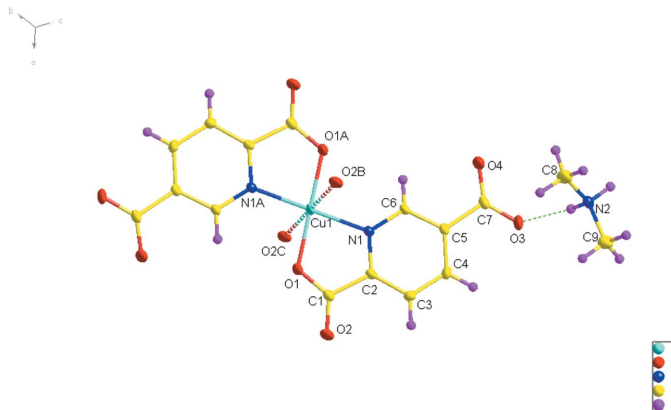


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. O1A/N1A and unlabelled atoms are related to O1/N1 and labelled atoms by the symmetry operation $(2 - x, 2 - y, -z)$. [Other symmetry codes: (B) $x - 1, y, z$; (C) $3 - x, 2 - y, -z$.]

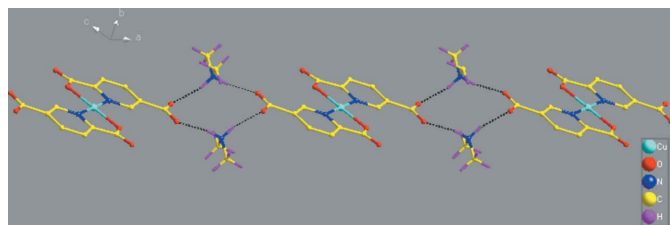


Figure 2
A view of the one-dimensional hydrogen-bonded chain along the $[11\bar{1}]$ direction.

$\text{Cu} \cdots \text{O2}^{\text{ii}}$ and $\text{Cu} \cdots \text{O2}^{\text{iii}}$ contacts of 2.821 (2) Å are ignored (Fig. 1). Selected bond lengths and angles are given in Table 1.

The dimethylammonium cations and the O atoms of the 5-carboxylate group of the pdc^{2-} ligand are connected *via* $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 2), forming one-dimensional chains along the $[11\bar{1}]$ direction.

Experimental

$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (1.0 mmol) and pyridine-2,5-dicarboxylic acid (1.0 mmol) were dissolved in dimethylformamide (10 ml). The solution was heated in a 25 ml Teflon-lined reaction vessel at 433 K for *ca* 3 d and then cooled to room temperature. Blue crystals of (I) were obtained in a yield of 68%. Elemental analysis, calculated for $\text{C}_{18}\text{H}_{22}\text{CuN}_4\text{O}_8$: C 44.49, H 4.56, N 11.53%; found: C 44.36, H 4.68, N 11.56%.

Crystal data

$(\text{C}_2\text{H}_8\text{N})_2[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)_2]$	$V = 485.8 (2) \text{ \AA}^3$
$M_r = 485.94$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.661 \text{ Mg m}^{-3}$
$a = 5.2516 (13) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.216 (2) \text{ \AA}$	$\mu = 1.18 \text{ mm}^{-1}$
$c = 12.290 (3) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\alpha = 103.232 (4)^\circ$	Block, blue
$\beta = 92.484 (4)^\circ$	$0.24 \times 0.14 \times 0.10 \text{ mm}$
$\gamma = 108.439 (4)^\circ$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	2504 measured reflections
φ and ω scans	1715 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1450 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.655$, $T_{\text{max}} = 1.000$ (expected range = 0.582–0.889)	$R_{\text{int}} = 0.021$ $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.0557P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
1715 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
144 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cu1–N1	1.965 (2)	Cu1–O2 ⁱ	2.821 (2)
Cu1–O1	1.952 (2)		
O1–Cu1–N1	83.44 (9)	O2 ⁱ –Cu1–N1	86.99 (8)
O1–Cu1–O2 ⁱ	97.55 (8)		

Symmetry code: (i) $x - 1, y, z$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N2}-\text{H2B} \cdots \text{O3}$	0.90	1.92	2.782 (3)	159
$\text{N2}-\text{H2A} \cdots \text{O4}^{\text{ii}}$	0.90	1.85	2.737 (3)	170

Symmetry code: (ii) $-x + 1, -y + 1, -z + 1$.

H atoms were positioned geometrically and treated as riding, with $\text{C}-\text{H} = 0.93-0.96 \text{ \AA}$ and $\text{N}-\text{H} = 0.90 \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$, or $1.5U_{\text{eq}}(\text{C})$ for methyl groups.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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