metal-organic papers

catena-Poly[[(2-methylimidazole)copper(II)]-μ-pyridine-2,6-dicarboxylato]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.056
wR factor = 0.136
Data-to-parameter ratio = 14.5

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

The reaction of pyridine-2,6-dicarboxylic acid (H$_2$DPC) and 2-methylimidazole (mim) with CuCl$_2$·6H$_2$O yields the one-dimensional title polymer, [Cu(C$_7$H$_3$O$_4$)(C$_4$H$_6$N$_2$)]$_n$. Hydrogen bonds connect the one-dimensional polymer chains into a three-dimensional supramolecular architecture.

Comment

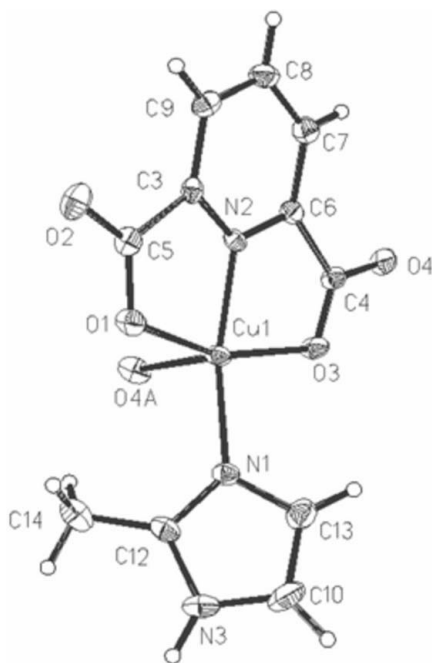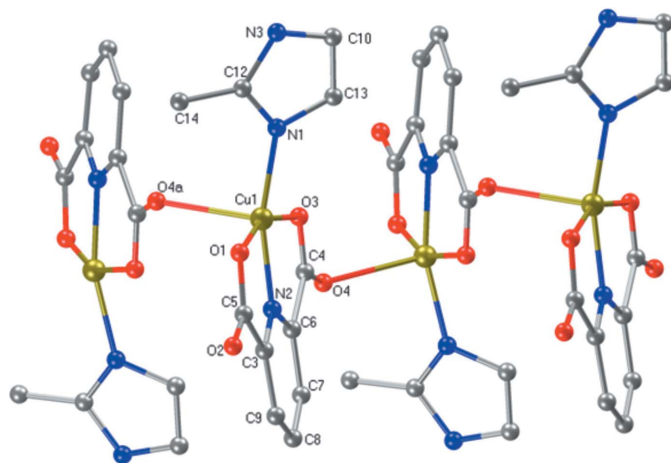Pyridine-2,6-dicarboxylic acid (H$_2$DPC) is an excellent ligand, not only due to the variety of coordination sites that it possesses but also due to its potential for hydrogen bonding *via* the carboxyl O atoms (MacDonald *et al.*, 2000). In particular, this ligand possesses two potential carboxylic acid coordination sites, which can be deprotonated resulting in a divalent anion, and a third, neutral aromatic nitrogen coordination site. Here we report the crystal structure of the title complex, (I), in which hydrogen bonds play an important role in the determination of the structure.

(I)
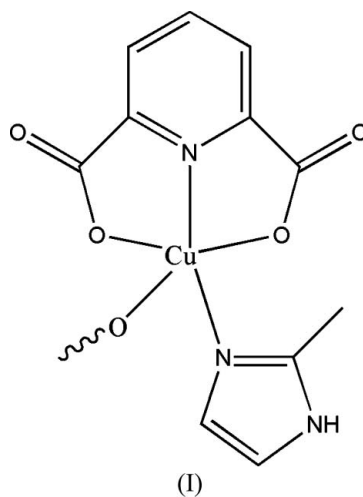
The asymmetric unit of (I) consists of a Cu^{II} ion, one pyridine-2,6-dicarboxylate (DPC) ion and one 2-methylimidazole (mim) unit, as shown in Fig. 1. The Cu^{II} center is surrounded by an N$_2$O$_3$ sphere in a distorted square-pyramidal geometry, of which one carbonyl O atom is from a neighbouring asymmetric unit. Two N atoms (N1 and N2) and two O atoms (O1 and O3) from the DPC and mim groups form the base of a square pyramid with a carboxyl O atom [O4A; symmetry code: (A) $1 - x$, $-y$, $\frac{1}{2} + z$] occupying the apical position. Two adjacent Cu^{II} ions are bridged by one carboxylate group and are separated by 5.66 (1) Å, thus forming a one-dimensional zigzag chain, as shown in Fig. 2. The Cu—N bond lengths [1.898 (3) and 1.938 (3) Å] are

the secondary amine group of the mim, forming hydrogen bonds (see Table 2), connecting neighbouring linear zigzag chains into a three-dimensional supramolecular architecture.

Experimental

A solution of H_2DPC (1 mmol, 0.167 g), $CuCl_2 \cdot 2H_2O$ (1 mmol, 0.174 g), mim (1 mmol, 0.082 g) and NaOH (2 mmol, 0.08 g) in 18 ml of methanol was heated in a 25 ml bomb at 413 K for 3 d, then cooled to room temperature at a rate of 5 K h^{-1}. Dark-green block-shaped crystals suitable for X-ray ananlysis were obtained in a yield of more than 35% based on the ligand H_2DPC. The product was washed with methanol and water, and then dried at ambient temperature. Elemental analysis found: C 42.30, H 2.88, N 13.60%; calculated: C 42.52, H 2.92, N 13.52%.

Crystal data

Figure 1
View of a fragment of polymeric (I), showing the coordination environment of the metal center and atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are drawn as spheres of arbitrary radius. [Symmetry code: (A) $1 - x, -y, \frac{1}{2} + z$.]

[Cu(C$_7$H$_3$O$_4$)(C$_4$H$_6$N$_2$)]	$Z = 4$
$M_r = 310.75$	$D_x = 1.775$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 15.490$ (3) Å	$\mu = 1.89$ mm^{-1}
$b = 11.021$ (2) Å	$T = 295$ (2) K
$c = 6.8124$ (14) Å	Block, dark green
$V = 1162.9$ (4) Å^3	$0.35 \times 0.21 \times 0.18$ mm

Data collection

Bruker APEX area-detector diffractometer	6787 measured reflections
	2516 independent reflections
φ and ω scans	2308 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.035$
	$\theta_{max} = 27.8°$
$T_{min} = 0.253$, $T_{max} = 0.365$ (expected range = 0.493–0.711)	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.8885P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.136$	$(\Delta/\sigma)_{max} = 0.017$
$S = 1.15$	$\Delta\rho_{max} = 0.93$ e Å^{-3}
2516 reflections	$\Delta\rho_{min} = -0.77$ e Å^{-3}
173 parameters	Absolute structure: Flack (1983), 1023 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.03 (3)

Figure 2
A view down [210], showing the one-dimensional chain running along the c axis. H atoms have been omitted.

comparable to those observed in other five-coordinate complexes and are well within the range of Cu—N distances noted in a previously reported complex (Xiang *et al.*, 2006). The Cu—O bond lengths in the basal sites [2.049 (4) and 2.013 (4) Å] are significantly shorter than the apical Cu—O4 distance [2.338 (4) Å], which reflects a weak axial interaction as expected for Jahn–Teller distorted copper(II) complexes.

In the crystal structure, complex (I) has a suprastructure based on C=O···H—N hydrogen-bond interactions. The uncoordinated carbonyl O atoms of the DPC ion interact with

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.898 (4)	Cu1—O3	2.050 (4)
Cu1—N1	1.941 (5)	O4—Cu1^i	2.343 (5)
Cu1—O1	2.011 (4)		
N2—Cu1—N1	164.0 (2)	N2—Cu1—O3	79.88 (16)
N2—Cu1—O1	80.60 (16)	N2—Cu1—O4^{ii}	101.46 (19)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{iii}	0.86	1.98	2.824 (7)	166

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

H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$; N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$] and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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