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catena-Poly[[(2,2′-bipyridine)copper(II)]-*μ*-5-nitroisophthalato]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.097
Data-to-parameter ratio = 14.7

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

In the title compound, $[Cu(C_8H_3NO_6)(C_{10}H_8N_2)]_n$, the Cu atom exists in a four-coordinate environment defined by two carboxyl O atoms belonging to two 5-nitroisophthalate dianions and two N atoms from a 2,2′-bipyridine molecule. The 5-nitroisophthalate dianion acts as a bridge between two Cu atoms in a tris-monodentate coordination mode, resulting in a zigzag coordination polymer.

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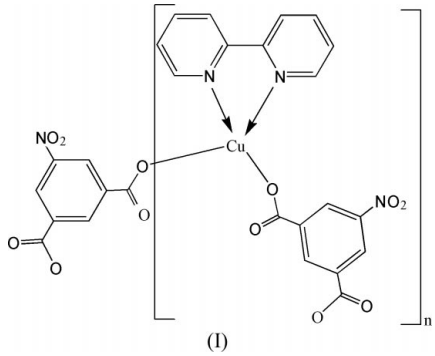
Comment

Following reports on the synthesis of one- and three-dimensional metal coordination polymers by using multicarboxylic acid ligands (Liu *et al.*, 2002; Lu *et al.*, 2001; O′Keeffe *et al.*, 2000; Yaghi *et al.*, 2003) such as terephthalic acid (Zhu *et al.*, 2004), isophthalic acid (Xiao *et al.*, 2004) and 1,2,4,5-benzenetetracarboxylic acid (Long *et al.*, 2003), we have used 5-nitroisophthalic acid in the synthesis of a coordination polymer, (I), of a copper(II) derivative in which the metal atom is chelated by 2,2′-bipyridine. The Cu^{II} atom has a four-coordinate environment defined by two carboxyl O atoms belonging to two 5-nitroisophthalate dianions and two N atoms from the heterocycle (Fig. 1); the geometry is square planar. The 5-nitroisophthalate dianion functions as a bridge between two Cu atoms, giving rise to a zigzag chain (Fig. 2). The motif is similar to those of $\{[Cu(phen)(phth)(H_2O)]\cdot H_2O\cdot DMF\}_n$ (phen is 1,10-phenanthroline and phth is isophthalate; Xiao *et al.*, 2004) and $\{[Cu(2,2'\text{-bipy})(tp)(H_2O)]\cdot H_2O\cdot DMF\}_n$ (tp is terephthalate and 2,2′-bipy is 2,2′-bipyridine; Xiao & Zhu, 2003). The structure differs in the mode of bonding as well as the deprotonation of the carboxyl groups of the 5-nitroisophthalate anion compared with those noted in $[CuCl(phen)_2]\cdot(C_8H_4NO_6)_2\cdot H_2O$ (Ye *et al.*, 2004). In (I), the two carboxyl groups are deprotoned and they are involved in coordination to the Cu atoms, whereas in $[CuCl(phen)_2]\cdot(C_8H_4NO_6)_2\cdot H_2O$, only one carboxyl group is deprotoned.



(I)

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of 5-nitroisophthalic acid (0.3 mmol), $Cu(CH_3COO)_2{\cdot}H_2O$ (0.3 mmol), 2,2-bipyridine (0.3 mmol) and water (8.0 ml) in a 15.0 ml telfon-lined stainless steel reactor. The solution was heated at 423 K for four days. After reaction, the vessel was slowly cooled to room temperature to give blue crystals.

Crystal data

$[Cu(C_8H_3NO_6)(C_{10}H_8N_2)]$	D_x = 1.728 Mg m^{-3}
M_r = 428.84	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3556 reflections
a = 9.5529 (11) Å	θ = 2.2–28.0°
b = 12.6089 (14) Å	μ = 1.37 mm^{-1}
c = 13.7463 (16) Å	T = 298 (2) K
β = 95.238 (2)°	Block, blue
V = 1648.8 (3) Å^3	0.30 × 0.22 × 0.13 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	3713 independent reflections
φ and ω scans	3266 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	R_{int} = 0.024
T_{min} = 0.684, T_{max} = 0.842	θ_{max} = 27.5°
9984 measured reflections	$h = -12 \rightarrow 12$
	$k = -7 \rightarrow 16$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.9168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.097	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
3713 reflections	
253 parameters	

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.9149 (17)	Cu1—N1	2.0046 (19)
Cu1—O3^{i}	1.9538 (16)	Cu1—N2	2.017 (2)
O2—Cu1—O3^{i}	98.71 (7)	O2—Cu1—N2	168.97 (8)
O2—Cu1—N1	91.11 (7)	O3^{i}—Cu1—N2	89.94 (7)
O3^{i}—Cu1—N1	170.18 (7)	N1—Cu1—N2	80.32 (8)

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

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

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

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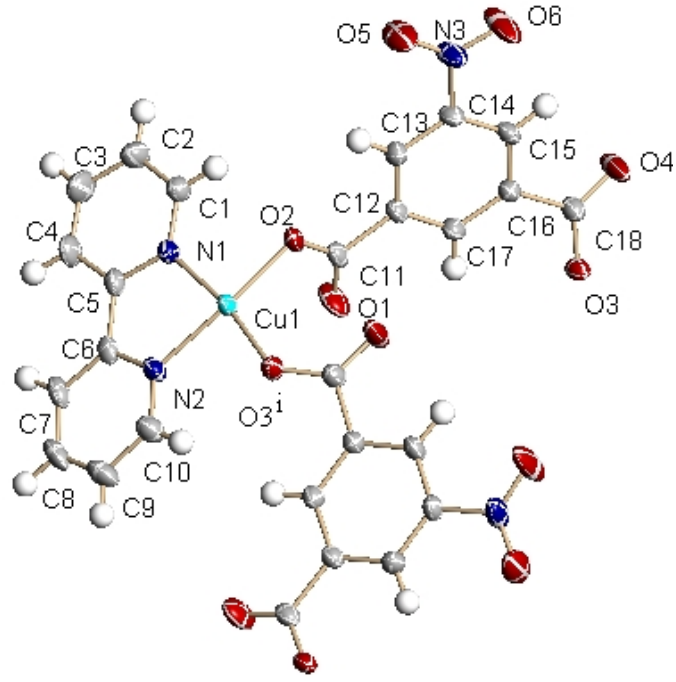

Figure 1
The coordination environment of the Cu atom in (I), with atom numbering, showing displacement ellipsoids at the 30% probability level [symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$].

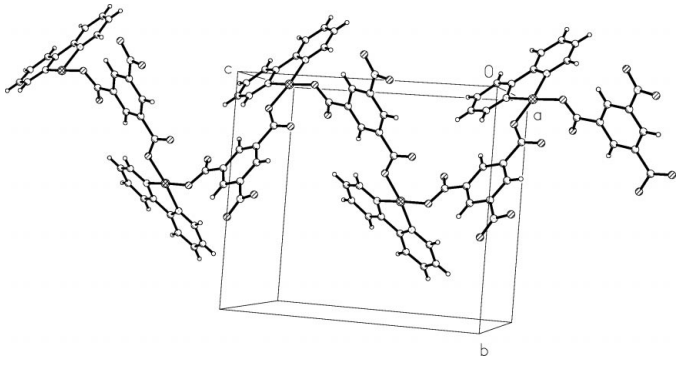

Figure 2
View of the zigzag chain of (I).

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