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catena-Poly[[bis(4-cyanobenzoato)-copper(II)]-μ-4,4′-bipyridine-κ^2N:N']

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.096
Data-to-parameter ratio = 13.0

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

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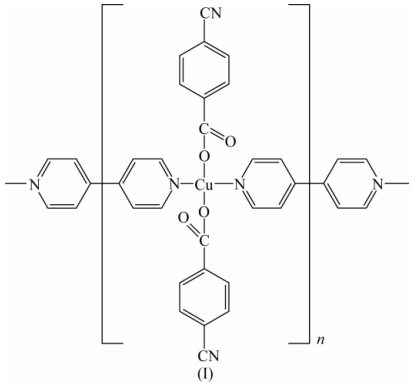
In the title polymeric complex, $[Cu(C_8H_4NO_2)_2(C_{10}H_8N_2)]_n$, the Cu^{II} center is located on an inversion center and surrounded by two N-donor molecules and two 4-cyanobenzoato ligands, which impose a square-planar environment on the metal. The spacer linker, 4,4′-bipyridine, is located on an inversion center and links adjacent metal atoms into a one-dimensional chain with a Cu···Cu separation of 11.218 (2) Å.

Comment

In recent years, much attention has been paid to the field of coordination polymers and has focused especially on the ligands of 4,4′-bipyridine, terephthalate and their derivatives, due to their potential applications in gas adsorption, ion exchange and heterogeneous catalysis (Eddaoudi *et al.*, 2002; Moulton & Zaworotko, 2001; Seo *et al.*, 2000). Complexes with 4-cyanobenzoic acid are sparse and a recent example suggests that this kind of complex has strong blue fluorescent emission (Yuan *et al.*, 2001). Moreover, a complex involving both 4-cyanobenzoic acid and 4,4′-bipyridine has not been reported so far. Here, we present the crystal structure of the Cu^{II} one-dimensional complex, the title compound, (I).



(I)

Compound (I) consists of a one-dimensional Cu^{II} complex in which the geometry around the Cu^{II} ion, located on an inversion center, is best described as square planar, as can be seen in Fig. 1. The coordination of the Cu atom is provided by two O atoms from two 4-cyanobenzoato ligands and two N atoms from two 4,4′-bipyridine ligands. Two benzoate groups and two pyridine rings of the 4,4′-bipyridine ligands are respectively located on opposite sides to minimize repulsion between the ligands. The Cu—O1 bond length [1.9176 (18) Å] is shorter than those of compounds such as $[Cu(py)_2(H_2O)(C_6H_5COO)_2]$ (Yang *et al.*, 2001) and $[Cu(C_6H_5COO)_2(2,2'\text{-bipy})]$ (Yang *et al.*, 1994). The 4-cyanobenzoate is coordinated, in monodentate fashion, to the copper center and the distance of Cu···O2 [2.861 (3) Å] is longer and is considered

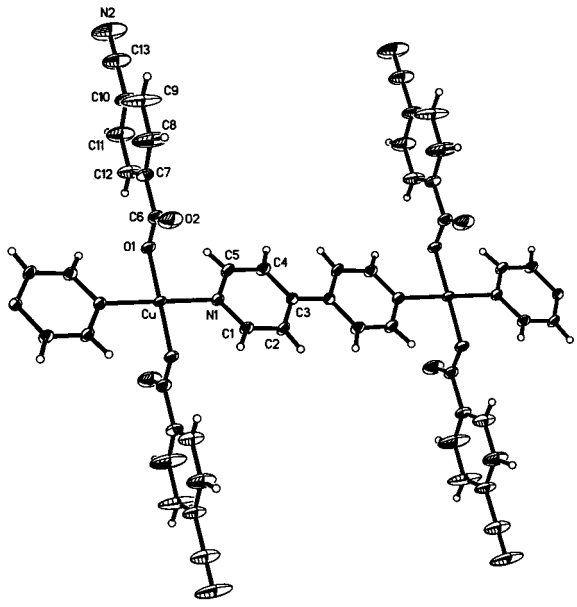


Figure 1
ORTEP diagram of (I), showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

as non-bonding. This coordination mode of the 4-cyanobenzoato ligand results in the four-coordinate copper geometry. The Cu—N1 bond length [2.051 (2) Å] is similar to those of $[Cu(py)_2(H_2O)(C_6H_5COO)_2]$ (Yang *et al.*, 2001) and $[Cu(C_6H_5COO)_2(2,2'\text{-bipy})]$ (Yang *et al.*, 1994) and those of Cu^{II} complexes with a 4,4′-bipyridine bridging linker (Xu *et al.*, 2002; Zhu & Kitagawa, 2002). The spacer ligand, 4,4′-bipyridine, located on an inversion center, links adjacent Cu atoms and extends the complex into a one-dimensional chain along $[1\bar{1}0]$ (Fig. 2). The Cu···Cu separation of the network is 11.218 (2) Å, which is the normal distance found in related copper–4,4′-bipyridine complexes. As expected, all other bond distances and angles are within normal ranges, and in good agreement with those of other 4,4′-bipyridine and carboxyl-containing complexes.

Experimental

The title complex, (I), was synthesized by a three-layered solution approach in a tube of *ca* 0.8 cm diameter with a length of 20 cm. The top layer was 10 ml of a methanol solution of 4,4′-bipyridine (0.2 mol l^{-1}) and 4-cyanobenzoic acid (0.05 mol l^{-1}). The middle layer was 3 ml of mixed solvents of methanol and water with volume ratio 1:1. The bottom layer was 5 ml of an aqueous solution of $Cu(NO_3)_2{\cdot}3H_2O$ (0.5 mol l^{-1}). After 3 d, crystals of (I) were obtained and filtered off.

Crystal data

$[Cu(C_8H_4NO_2)_2(C_{10}H_8N_2)]$	$Z = 1$
$M_r = 511.97$	$D_x = 1.507$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 5.3279$ (10) Å	Cell parameters from 978 reflections
$b = 8.9739$ (17) Å	$\theta = 5.3$–$48.0°$
$c = 12.195$ (2) Å	$\mu = 1.01$ mm^{-1}
$\alpha = 99.734$ (3)°	$T = 293$ (2) K
$\beta = 92.495$ (4)°	Plate, blue
$\gamma = 100.190$ (4)°	0.31 × 0.11 × 0.04 mm
$V = 563.99$ (18) Å^3	

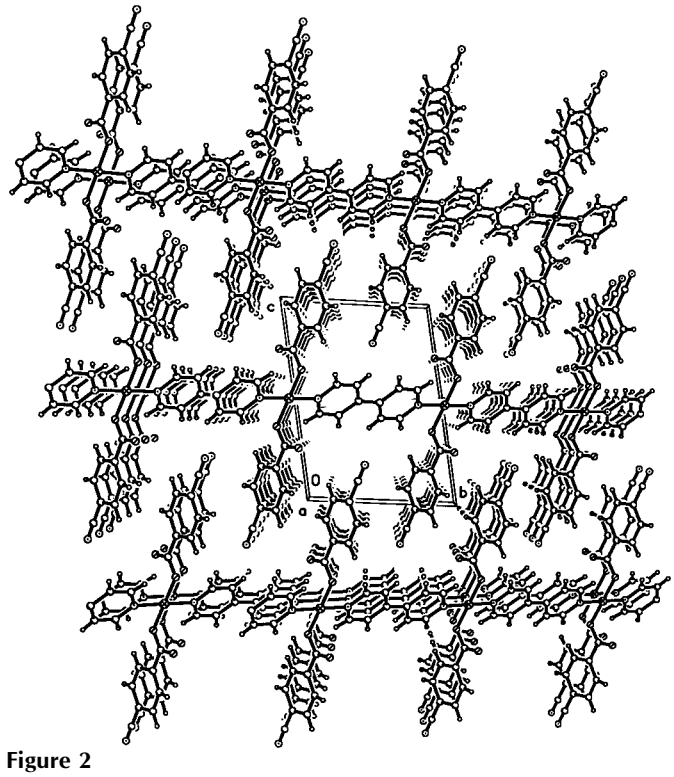


Figure 2
View of the packing in the title complex (I).

Data collection

Bruker SMART CCD area-detector diffractometer	2504 independent reflections
	2053 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 28.3°$
	$h = -7 \rightarrow 6$
$T_{min} = 0.820$, $T_{max} = 0.965$	$k = -11 \rightarrow 8$
3490 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	
$S = 0.95$	$(\Delta/\sigma)_{max} = 0.042$
2504 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
192 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.9176 (18)	C1—C2	1.365 (4)
Cu—N1	2.051 (2)	C2—C3	1.380 (4)
O1—C6	1.277 (4)	C3—C4	1.393 (3)
O2—C6	1.214 (4)	C3—C3^{i}	1.478 (5)
N1—C5	1.341 (3)	C4—C5	1.369 (4)
N1—C1	1.347 (3)		
O1—Cu—N1	90.17 (8)	O2—C6—O1	124.6 (3)
C6—O1—Cu	114.5 (2)		

Symmetry code: (i) $2-x, 1-y, 1-z$.

The completeness of the data collection was relatively low (90.1%), although all parameters were set according to the suggestions of *SMART* (Bruker, 1997). The H atoms were refined isotropically, with C—H bond lengths 0.89 (4)–0.92 (2) Å. The atomic displacement parameters of N2, C8 and C9 are abnormal. Their displacement ellipsoids are very elongated, suggesting some unresolved disorder.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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