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catena-Poly[bis(4-chlorobenzoato)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) = 0.004 Å
R factor = 0.037
wR factor = 0.095
Data-to-parameter ratio = 16.6

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

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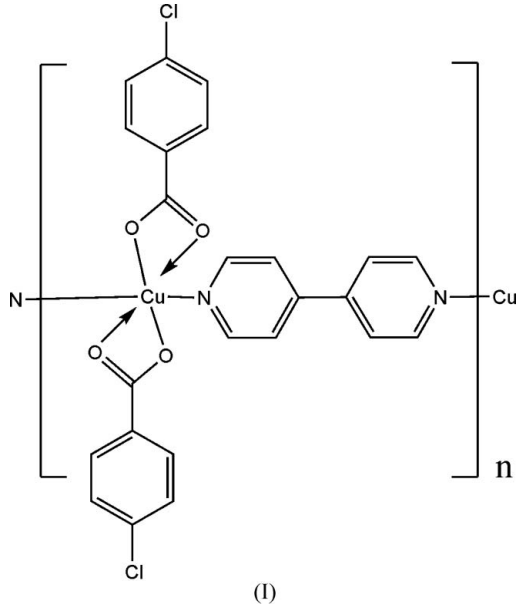
In the title complex, $[Cu(C_7H_4ClO_2)_2(C_{10}H_8N_2)]_n$, the Cu^{II} ion, lying on an inversion centre, is coordinated by two monodentate 4-chlorobenzoate ligands and two N atoms from two bridging 4,4′-bipyridine ligands, each disposed about a centre of inversion, within an N_2O_2 square plane. This coordination leads to the formation of a linear chain.

Comment

The self-assembly of molecular building blocks containing organic ligands and inorganic metal ions provides an efficient and reliable approach for the design and synthesis of organic–inorganic hybrid materials (Draper *et al.*, 2004; Li *et al.*, 2005). In recent years, many copper(II) complexes have been generated for their tunable properties such as molecular recognition, adsorption and separation processes, catalysis, ion exchange and as molecular magnets (Kitagawa *et al.*, 2004; Min & Suh, 2000). Here, a new copper(II) complex, (I), is reported.



(I)

In (I), the Cu^{II} ion, lying on an inversion centre, is coordinated by two O atoms from two 4-chlorobenzoate ligands and two N atoms derived from symmetry-related 4,4′-bipyridine ligands, each disposed about a centre of inversion. The resulting coordination geometry is based on N_2O_2 square planar (Fig. 1). The Cu—O and Cu—N distances (Table 1) are comparable with literature values (Phillips & Lee, 2001). In addition, there are weak intramolecular Cu···O2 interactions (Falvello *et al.*, 2001) of 2.743 (2) Å above and below the

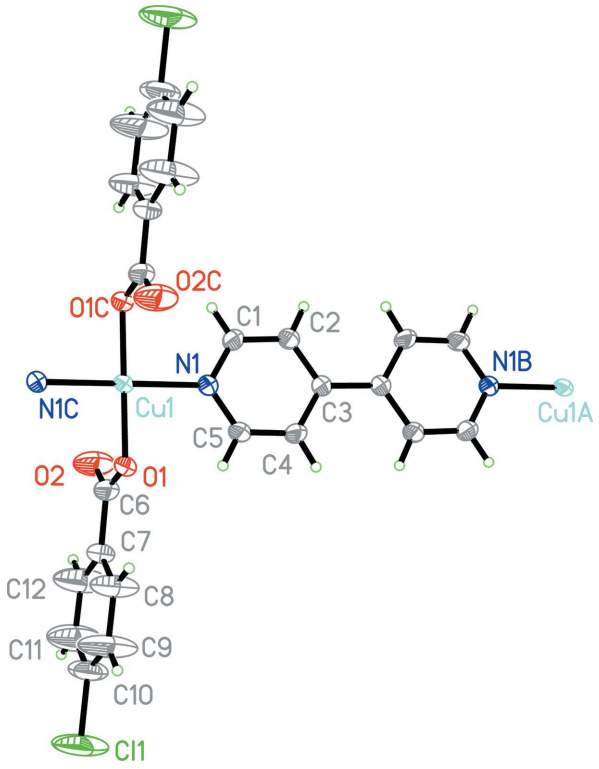


Figure 1
Part of the polymeric structure of the title complex, with displacement ellipsoids drawn at the 50% probalility level. [Symmetry codes: (A) $-1+x, 1+y, z$; (B) $-x, 1-y, -z$; (C) $1-x, -y, -z$.]

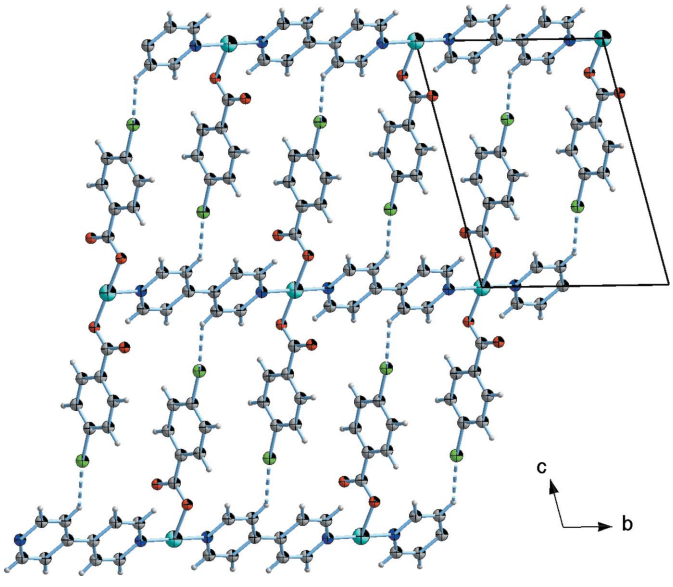


Figure 2
A view of the chains in (I), extended by C–H···Cl interactions (dashed lines) along the *a* axis into a two-dimensional array.

square plane. The 4,4′-bipyridine ligands connect the $\{Cu(C_7H_4ClO_2)_2\}$ units to form an infinite one-dimensional chain (Fig. 2). The chains are linked into a two-dimensional array *via* intermolecular $Cl1\cdots H4^{i}—C4^{i}$ interactions, with $Cl1\cdots H4^{i}—C4^{i} = 2.86$ Å, $Cl1\cdots C4^{i} = 3.541$ (3) Å and an angle of 131° at $H4^{i}$ (Fig. 2) [symmetry code: (i) $2-x, 1-y, 1-z$].

Experimental

A mixture of CuO (0.5 mmol, 0.04 g), 4,4′-bipyridine (0.5 mmol, 0.096 g), 4-chlorobenzoic acid (1 mmol, 0.16 g) and H_2O (5 ml) was placed in a 25 ml acid-digestion bomb at 413 K for 3 d. After cooling to room temperature (5 K h^{-1}), purple crystals were obtained (yield 60% based on Cu; m.p. 568 K). These were filtered off, washed with ethanol and dried in air. Elemental analysis calculated (%): C 54.30, H 3.04, N 5.28; found: C 54.62, H 2.86, N 5.21.

Crystal data

$[Cu(C_7H_4ClO_2)_2(C_{10}H_8N_2)]$
$M_r = 530.83$
Triclinic, $P\overline{1}$
$a = 5.4005$ (11) Å
$b = 8.9359$ (18) Å
$c = 12.019$ (2) Å
$\alpha = 103.17$ (3)°
$\beta = 94.31$ (3)°
$\gamma = 100.11$ (3)°
$V = 551.97$ (18) Å^3
$Z = 1$
$D_x = 1.597$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.27$ mm^{-1}
$T = 293$ (2) K
Block, purple
0.48 × 0.31 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.583$, $T_{max} = 0.856$
5484 measured reflections
2510 independent reflections
2325 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.095$
$S = 1.07$
2510 reflections
151 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.1853P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9286 (16)	C6—O1	1.276 (3)
Cu1—N1	2.0632 (16)	C6—O2	1.223 (3)
O1—Cu1—N1	90.03 (7)	$O1^{i}$—Cu1—N1	89.97 (7)

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

H-atom parameters were refined in the riding-model approximation, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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