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catena-Poly[[(di-2-pyridylamine-κ^2N,N')copper(II)]-μ-benzene-1,4-dicarboxylato-$\kappa^4O,O':O'',O'''$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.118
Data-to-parameter ratio = 15.3

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

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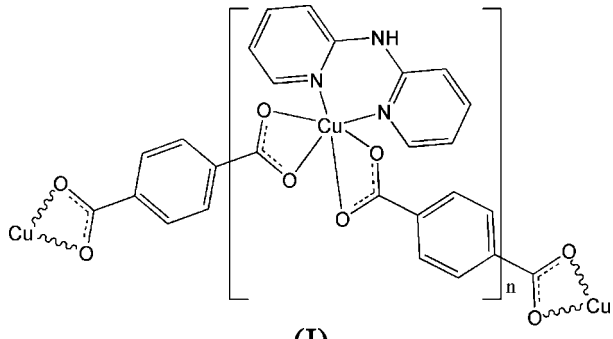
In the title complex, $[Cu(C_8H_4O_4)(C_{10}H_9N_3)]_n$, the benzene-1,4-dicarboxylate dianions bridge the Cu^{II} atoms to form polymeric complex chains. The Cu^{II} atom has a distorted octahedral coordination geometry. The centroid-to-centroid separation of 3.932 (2) Å indicates π–π stacking between nearly parallel pyridine rings.

Comment

Metal complexes with both benzene-1,4-dicarboxylate (tpht) and 2,2′-bipyridylamine (bipya) ligands have been reported recently, namely $[Cu(tpht)(bipya)]\cdot H_2O$ (Karanović *et al.*, 2002) and $[M(tpht)(bipya)(H_2O)_2]\cdot 3H_2O$ (M = Co or Ni) (Rogan *et al.*, 2000). Here, we report the structure of the title Cu^{II} complex, (I), with these ligands.



(I)

A segment of the polymeric molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom is coordinated by two tpht ligands and one bipya ligand in a distorted octahedral geometry (Table 1). The tpht dianions bridge the Cu^{II} atoms to form zigzag chains in the crystal structure, similar to a previously reported structure (Karanović *et al.*, 2002).

The centroid-to-centroid separation of 3.932 (2) Å between nearly parallel N1- and N2^{ii}-containing pyridine rings [dihedral angle 7.92 (6)°] indicates the existence of weak π–π stacking between bipya ligands [symmetry code: (ii) $1-x, -y, 1-z$].

Experimental

A mixture of $Cu(ClO_4)_2\cdot 6H_2O$ (0.186 g, 0.5 mmol), benzene-1,4-dicarboxylic acid (0.083 g, 0.5 mmol), 2,2′-bipyridylamine (0.085 g, 0.5 mmol), Na_2CO_3 (0.055 g, 0.5 mmol) and water (10 ml) was sealed in a 15 ml Teflon-lined stainless steel reactor and heated at 423 K for 60 h, to yield single crystals of (I).

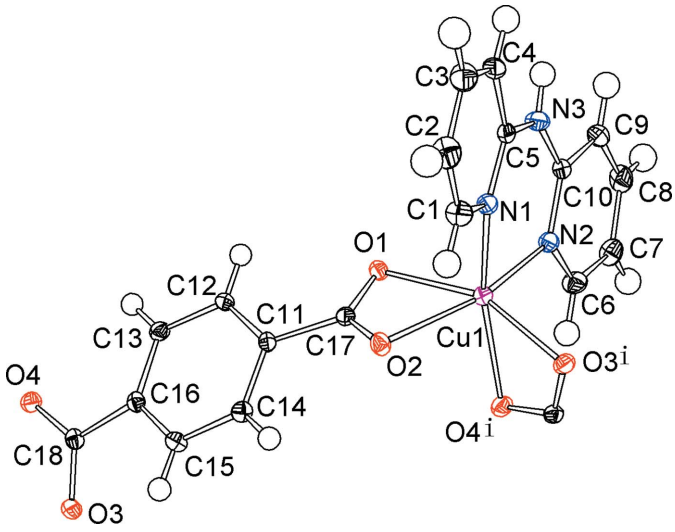


Figure 1
Part of the structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry code: (i) $1 + x, \frac{1}{2} - y, \frac{1}{2} + z$.]

Crystal data

$[Cu(C_8H_4O_4)(C_{10}H_9N_3)]$
$M_r = 398.86$
Monoclinic, $P2_1/c$
$a = 7.6403$ (6) Å
$b = 21.103$ (2) Å
$c = 9.8015$ (8) Å
$\beta = 96.066$ (4)°
$V = 1571.5$ (2) Å^3
$Z = 4$
$D_x = 1.686$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.42$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.20 × 0.15 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.743$, $T_{max} = 0.810$
12092 measured reflections
3592 independent reflections
3069 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.118$
$S = 1.09$
3592 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 2.0459P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.022 (2)	Cu1—O2	2.168 (2)
Cu1—N2	2.047 (3)	Cu1—O3^{i}	2.056 (2)
Cu1—O1	2.106 (2)	Cu1—O4^{i}	2.171 (2)

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

All H atoms were placed in calculated positions, with C—H = 0.93 and N—H = 0.86 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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