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catena-Poly[[aqua(pyrazino[2,3-*f*][1,10]-phenanthroline-κ^2N,N')copper(II)]-μ-benzene-1,4-dicarboxylato-κ^2O^1:O^4]

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.122
Data-to-parameter ratio = 14.3

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

In the title compound, $[Cu(C_8H_4O_4)(C_{14}H_8N_4)(H_2O)]_n$, the Cu^{II} atom is five-coordinate and exhibits a distorted square-pyramidal coordination geometry. The benzene-1,4-dicarboxylate ligand bridges the Cu^{II} atoms to form a one-dimensional chain structure.

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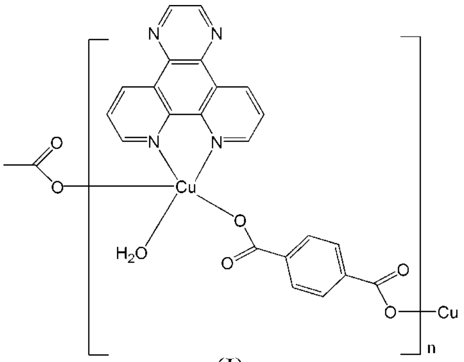
Comment

Coordination polymers constructed using dicarboxylates and heteroaromatic *N*-donor chelating ligands are of special interest. 1,10-Phenanthroline (phen) has been widely used in the construction of metal-organic complexes (Chen & Liu, 2002). Pyrazino[2,3-*f*][1,10]phenanthroline (*L*) as a phen derivative possesses an extended aromatic system. We employed benzene-1,4-dicarboxylic acid (1,4-H_2bdc) as a linker and *L* as a secondary chelating ligand to prepare a new coordination polymer, $[Cu(1,4\text{-bdc})(L)(H_2O)]_n$, (I).



(I)

In compound (I), each Cu^{II} atom is five-coordinate and exhibits a distorted square-pyramidal coordination geometry (Fig. 1). One carboxylate O atom (O1), one water molecule (O1*W*) and two N atoms (N1 and N2) from the *L* ligand form the basal plane, whereas a carboxylate atom O3 from a 1,4-bdc ligand at $(\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z)$ occupies the apical position with a Cu1—O3 distance of 2.2311 (19) Å. The Cu^{II} atoms are bridged by 1,4-bdc ligands to generate a one-dimensional chain structure. There are π–π interactions between phenanthroline of the *L* ligands in neighboring chains [C1–C14/N1–N4 at (*x*, *y*, *z*) and (1 − *x*, −*y*, −*z*)], with a shortest atom-to-atom distance of 3.471 (5) Å. O—H⋯O hydrogen bonds between the water molecules and carboxylate O atoms complete the crystal structure of (I) (Table 1).

Experimental

L was synthesized according to the reported method (Dickeson & Summers, 1970). A methanol solution (18 ml) of *L* (0.120 g, 0.5 mmol) was mixed with an aqueous solution (12 ml) of $CuCl_2 \cdot 2H_2O$ (0.086 g, 0.5 mmol) with stirring at 383 K. The resulting solution was filtered, the filtrate was allowed to stand in air at room temperature for one week, and blue crystals of (I) were obtained (yield 46% based on Cu).

Crystal data

$[Cu(C_8H_4O_4)(C_{14}H_8N_4)(H_2O)]$
$M_r = 477.91$
Monoclinic, $P2_1/n$
$a = 11.489\ (2)$ Å
$b = 15.054\ (3)$ Å
$c = 12.186\ (2)$ Å
$\beta = 116.40\ (3)^\circ$
$V = 1887.8\ (8)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.20$ mm^{-1}
$T = 292\ (2)$ K
$0.33 \times 0.29 \times 0.21$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.663$, $T_{max} = 0.775$
17593 measured reflections
4258 independent reflections
3427 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.122$
$S = 1.07$
4258 reflections
297 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H11*W*···O2	0.84 (4)	1.83 (3)	2.593 (3)	151 (5)
O1*W*—H12*W*···O4^{i}	0.85 (2)	1.739 (19)	2.585 (3)	173 (4)

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms on the C atoms were positioned geometrically and refined as riding, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms on water molecule were located in a difference Fourier map and refined isotropically with a distance restraint of O—H = 0.85 (2) Å.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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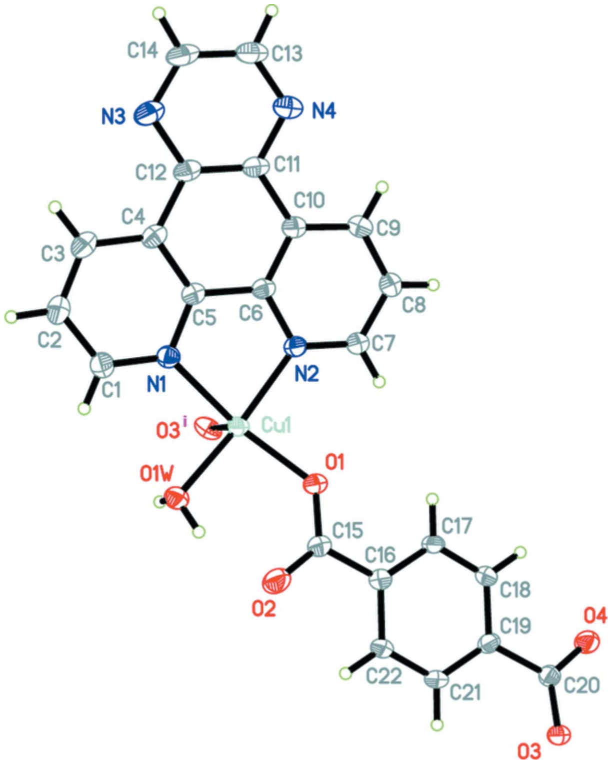

Figure 1
The asymmetric unit of (I), extended to show the complete coordination of copper. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$.]

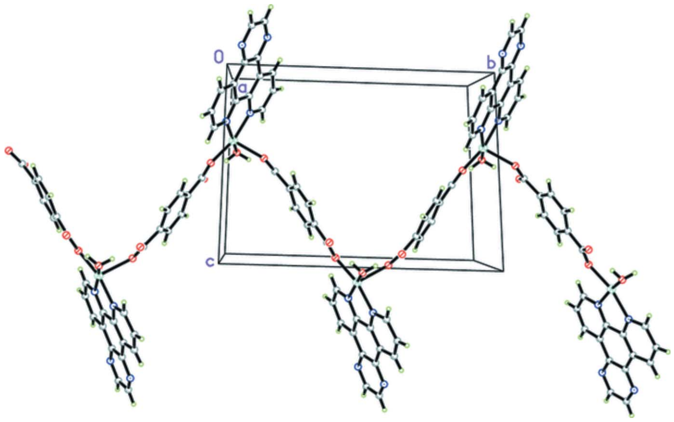

Figure 2
View of the chain structure of (I).

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