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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
 Disorder in main residue  
 R factor = 0.050  
 wR factor = 0.144  
 Data-to-parameter ratio = 13.3

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

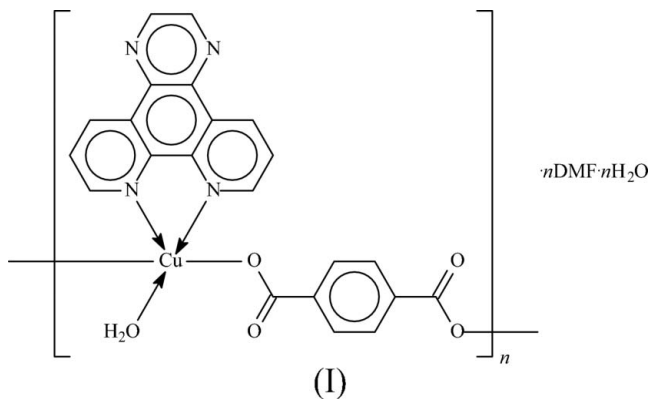
**catena-Poly[[[aqua(pyrazino[2,3-*f*][1,10]phenanthroline- $\kappa^2N,N'$ )copper(II)]- $\mu$ -terephthalato- $\kappa^2O:O'$ ] *N,N*-dimethylformamide monohydrate]**

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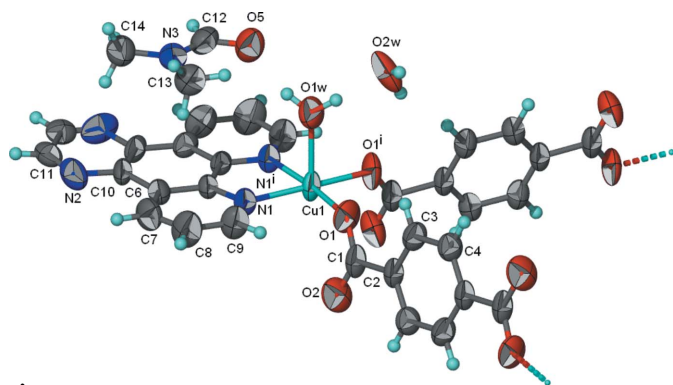
In the title compound,  $[\text{Cu}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{14}\text{H}_8\text{N}_4)(\text{H}_2\text{O})] \cdot \text{C}_3\text{H}_7\text{NO} \cdot \text{H}_2\text{O}$ , the  $\text{Cu}^{\text{II}}$  atom binds a water molecule and is chelated by the pyrazinophenanthroline *N*-heterocycle. It is also linked covalently to a terephthalate dianion that lies on a special position of  $\bar{1}$  site symmetry. This dianion serves as a spacer to connect adjacent square-pyramidal metal atoms into a helical chain that propagates along the *b* axis of the monoclinic unit cell. The chain motif is consolidated into a layer structure by hydrogen bonds involving the coordinated and uncoordinated water molecules. The Cu atom and the coordinated water molecule lie on a mirror plane, while the *N*-heterocycle, the disordered uncoordinated water molecule and disordered dimethylformamide solvent molecule lie about a mirror plane.

**Comment**

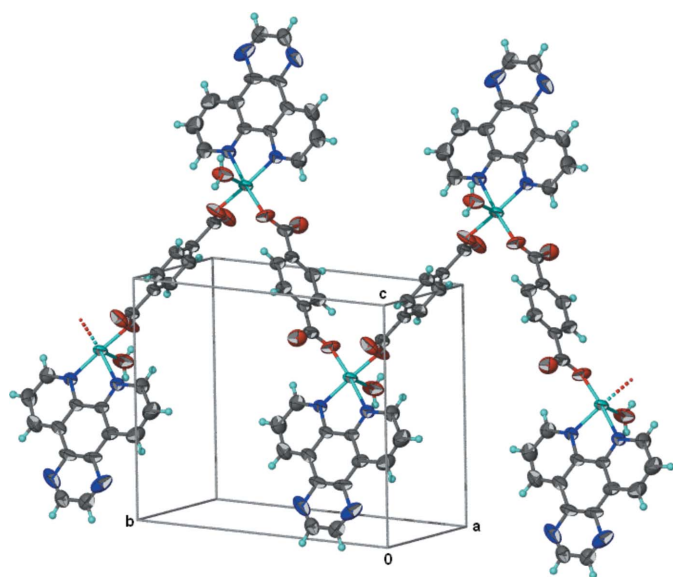
There have been several crystal structure studies of polymeric complexes of copper(II) terephthalate in which the Cu atom is chelated by 2,2'-bipyridine (Bu *et al.*, 2003; Huang *et al.*, 2003; Xiao & Zhu, 2003; Yang & Li, 2005; Yang *et al.*, 2003). As the terephthalate unit is necessarily inflexible, it would function as a rigid bridging dicarboxylate ligand. The present attempt at synthesizing a copper terephthalate complex with pyrazino[2,3-*f*][1,10]phenanthroline in place of 2,2'-bipyridine gave the title complex,  $[(\text{H}_2\text{O})(\text{C}_{14}\text{H}_8\text{N}_4)(\text{C}_8\text{H}_4\text{O}_4)\text{Cu}] \cdot \text{DMF} \cdot \text{H}_2\text{O}$ , (I) (DMF is dimethylformamide). The ligand itself can be synthesized hydrothermally in high yield (Che, Li *et al.*, 2006). This report complements a recent study of the copper(II) fumarate complex of this *N*-heterocycle (Che, Liu & Xu, 2006).



Compound (I) crystallizes with solvent DMF and water molecules (Fig. 1). The terephthalate lies on a special position of site symmetry  $\bar{1}$ . The Cu atom and the coordinated water



**Figure 1**  
Part of the polymeric chain structure of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as spheres of arbitrary radii. [Symmetry code (i):  $x, \frac{1}{2} - y, z$ .]



**Figure 2**  
The chain structure of (I). The DMF and solvent water molecules are not shown.

molecule lie on a mirror plane, while the *N*-heterocycle, the disordered uncoordinated water molecule and disordered dimethylformamide solvent molecule lie about a mirror plane. The Cu atom is chelated by the sterically crowded *N*-heterocycle, and is also coordinated by a water molecule. The square-pyramidal coordination environment is completed by bonds to the carboxylate O atoms of two terephthalate dianions. These terephthalate spacers result in the formation of a helical chain (Fig. 2) and these chains are consolidated into layers by hydrogen bonds that involve the solvent water and DMF molecules (Table 2).

## Experimental

A methanol solution (4 ml) of pyrazino[2,3-*f*][1,10]phenanthroline (59 mg, 0.25 mmol) was mixed with an aqueous solution (4 ml) of copper(II) chloride dihydrate (43 mg, 0.25 mmol). A DMF solution (18 ml) of terephthalic acid (42 mg, 0.25 mmol) was added and the mixture heated at 348 K for 5 h. The solution was then filtered and

blue crystals of (I) separated from the solution after several days in 60% yield.

## Crystal data

$[\text{Cu}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{14}\text{H}_8\text{N}_4)(\text{H}_2\text{O})] \cdot$   
 $\text{C}_3\text{H}_7\text{NO} \cdot \text{H}_2\text{O}$   
 $M_r = 569.02$   
Monoclinic,  $P2_1/m$   
 $a = 7.275$  (4) Å  
 $b = 13.970$  (5) Å  
 $c = 11.794$  (5) Å  
 $\beta = 92.78$  (2)°

$V = 1197$  (1) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.578$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.97$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Block, green  
 $0.21 \times 0.19 \times 0.10$  mm

## Data collection

Rigaku R-AXIS RAPID IP  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.701$ ,  $T_{\max} = 0.909$

11896 measured reflections  
2856 independent reflections  
2229 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$   
 $\theta_{\max} = 27.5^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.144$   
 $S = 1.08$   
2856 reflections  
214 parameters  
H atoms treated by a mixture of  
independent and constrained  
refinement

$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 0.8938P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.85$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.56$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O1	1.934 (2)	Cu1—O1w	2.279 (4)
Cu1—N1	2.028 (3)		
O1—Cu1—O1 <sup>i</sup>	90.5 (2)	O1—Cu1—N1 <sup>i</sup>	174.7 (1)
O1—Cu1—O1w	91.8 (2)	O1w—Cu1—N1	90.6 (1)
O1—Cu1—N1	94.1 (1)	N1—Cu1—N1 <sup>i</sup>	81.1 (1)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1w—H1w1...O5	0.84 (1)	2.01 (1)	2.708 (7)	140 (1)
O1w—H1w2...O2w	0.85 (1)	1.87 (1)	2.716 (7)	175 (3)
O2w—H2w1...O2 <sup>ii</sup>	0.85 (1)	1.77 (5)	2.61 (4)	167 (9)

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

The structure is disordered over a mirror plane in the pyrazino-phenanthroline, DMF and solvent water parts of the asymmetric unit. For the  $\text{C}_{14}\text{H}_8\text{N}_4$  ligand, the N—C distances were restrained to 1.35 (1) Å and the C—C distances to 1.39 (1) Å; the ligand was also restrained to near-planarity. For the DMF molecule, the following distance restraints were imposed: C12—O5 = 1.25 (1) Å, C12—N3 = 1.35 (1) Å, C13—N3 = C14—N3 = 1.45 (1) Å, C12...C13 = C12...C14 = 2.43 (2) Å, C13...C14 = 2.51 (2) Å and O5...N3 = 2.25 (2) Å. The molecule was also restrained to be approximately planar, and the atoms were restrained to vibrate in a nearly isotropic manner. The solvent water molecule was allowed to refine off the mirror plane.

Carbon-bound H atoms were geometrically geometrically, with C–H = 0.93–0.96 Å, and were included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ . The methyl groups were rotated to fit the electron density. Water H atoms were located in a difference Fourier map and were refined with distance restraints of O–H = 0.85 (1) Å and H··H = 1.39 (1) Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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