metal-organic papers

catena-Poly[[[aqua(1,10-phenanthroline)copper(II)]-μ-isophthalato] N,N-dimethylformamide solvate monohydrate]

Hong-Ping Xiao,* Xin-Hua Li and Mao-Lin Hu

Department of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou, 325027, People's Republic of China

Correspondence e-mail: hp_xiao@wznc.zj.cn

In the title complex, $\{[Cu(C_8H_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot C_3H_7NO\cdot H_2O\}_n$, the Cu atom is surrounded by two O atoms from two isophthalate dianions, an aqua O atom and two N atoms from a phenanthroline heterocycle in a distorted square-pyramidal geometry. The isophthalate dianion functions as a bridge between two Cu atoms and generates a one-dimensional zigzag chain coordination polymer.

Comment

Among the metal complexes of terephthalic acid (H_2ta) and its derivatives (Cano *et al.*, 1997; Liu *et al.*, 2004; Otto & Wheeler, 2001; Tan *et al.*, 1997), the copper–phenanthroline (phen) system has been well studied and displays a diversity of structures; examples include two dimeric complexes, $[Cu_2(ta)(phen)_4](ClO_4)_2$ and $[Cu_2Cl_2(ta)(phen)_2(H_2O)_2]$, and three polymeric complexes, $[Cu(ta)(phen)]$, $[Cu(ta)(phen)(H_2O)]$ and $[Cu(ta)(phen)(H_2O)]\cdot H_2O\cdot DMF$ (Sun *et al.*, 2000, 2001; Xiao *et al.*, 2004; Zhu *et al.*, 2004). The title compound, $[Cu(phen)(phth)(H_2O)]\cdot H_2O\cdot DMF$, (I), where terephthalic acid is replaced by isophthalic acid (H_2phth), is a one-dimensional zigzag chain coordination polymer.

(I)
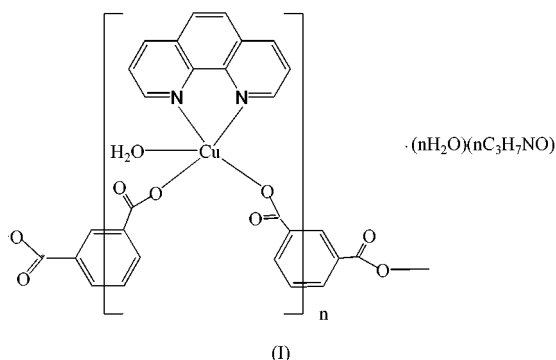
In (I), the Cu atom is surrounded by two O atoms from two isophthalate dianions, an aqua O atom and two N atoms from a phenanthroline heterocycle in a distorted square-pyramidal geometry (Fig. 1). The apical position is occupied by the aqua O atom, the corresponding axial bond distance [2.309 (2) Å] being longer than the two equatorial Cu—O(carboxylate) bonds distances [1.940 (2) Å and 1.965 (2) Å]. The isophthalate dianion functions as a bridge between two Cu atoms in a bis-monodentate coordination mode. The 1,10-phenanthroline acts as a chelate ligand. A one-dimensional zigzag chain is formed by the Cu^{II} cations, the μ_2-bridging isophthalate dianions, the aqua molecules and the terminal 1,10-phenanthroline ligands (Fig. 2), which is similar to the structure of the complex, $[Cu(phen)(ta)(H_2O)]\cdot H_2O\cdot DMF$ (Zhu *et al.*, 2004).
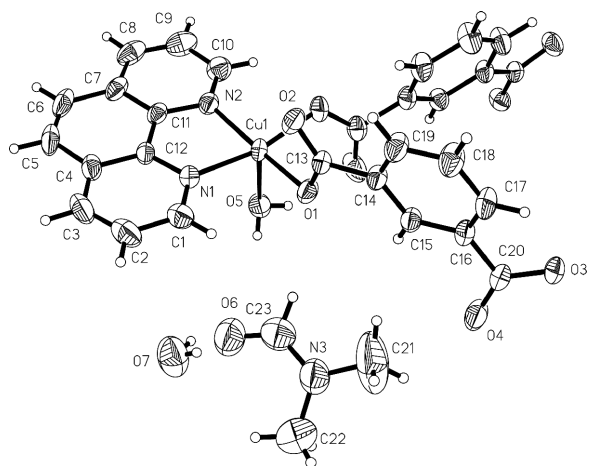
Figure 1
The asymmetric unit of (I), together with the symmetry-related coordinated isophthalate ligand. The independent non-H atoms are labelled, and displacement ellipsoids are drawn at the 50% probability level.
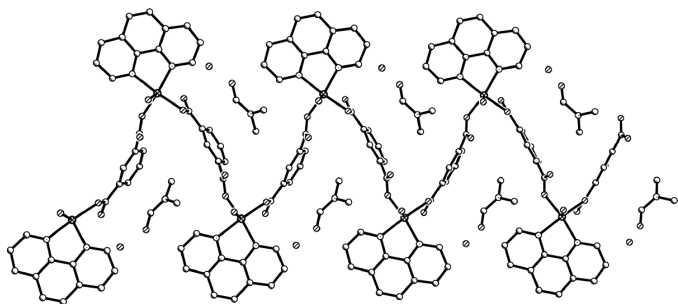

Figure 2
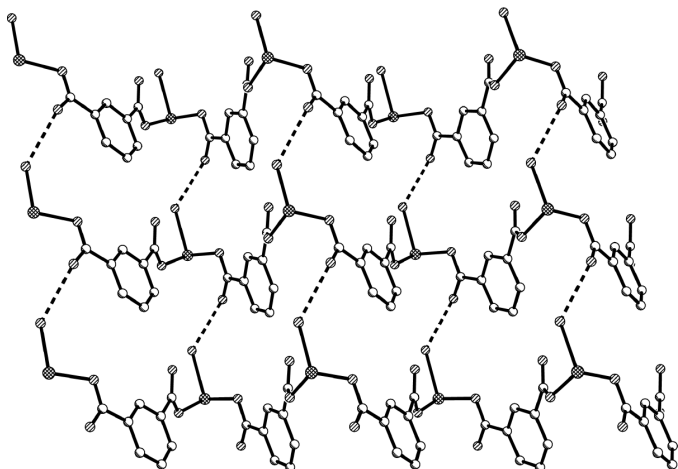View of the one-dimensional zigzag chain in (I). H atoms have been omitted.

Figure 3
View of the two-dimensional hydrogen-bonding network in (I). The 1,10-phenanthroline ligands, the DMF and water solvent molecules, and H atoms have been omitted for clarity.

An O5—H5B$\cdots$O2^i [symmetry code: (i) $x + 1$, y, z] inter-molecular hydrogen bond is formed between neighbouring one-dimensional zigzag chains, resulting in a two-dimensional network (Fig. 3). Moreover, there are π–π interactions of the 1,10-phenanthroline heterocycle belonging to adjacent zigzag chains. This leads from a two-dimensional network to a three-

dimensional network with cavities. The DMF and water solvent molecules are embedded in the cavities.

Experimental

A solution (10 ml) of dimethylformamide containing $Cu_2Cl_2\cdot2H_2O$ (0.5 mol, 0.085 g) and isophthalic acid (0.5 mmol, 0.083 g) was added slowly to a solution (10 ml) of dimethylformamide containing 1,10-phenanthroline (0.5 mmol, 0.099 g). The mixture was stirred for a few minutes and left to stand at room temperature for about four months, after which time blue crystals were obtained.

Crystal data

$[Cu(C_8H_4O_4)(C_{12}H_8N_2)(H_2O)]\cdot$ $C_3H_7NO\cdot H_2O$	$D_x = 1.496$ Mg m^{-3}
$M_r = 516.98$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 654
$a = 6.9009$ (2) Å	reflections
$b = 31.1833$ (9) Å	$\theta = 2.4$–23.0°
$c = 10.7808$ (3) Å	$\mu = 1.00$ mm^{-1}
$\beta = 98.312$ (1)°	$T = 293$ (2) K
$V = 2295.58$ (11) Å^3	Prism, blue
$Z = 4$	$0.45 \times 0.38 \times 0.27$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	4037 independent reflections
	3652 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.020$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{max} = 25.0°$
	$h = -8 \rightarrow 8$
$T_{min} = 0.635$, $T_{max} = 0.764$	$k = -36 \rightarrow 27$
11975 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$+ 1.5778P]$
$wR(F^2) = 0.117$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
4037 reflections	$\Delta\rho_{max} = 0.81$ e Å^{-3}
311 parameters	$\Delta\rho_{min} = -0.74$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.0009 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—O3^i	1.9400 (18)	Cu1—N2	2.029 (2)
Cu1—O1	1.9650 (18)	Cu1—O5	2.309 (2)
Cu1—N1	2.006 (2)		
O3^i—Cu1—O1	89.04 (8)	N1—Cu1—N2	81.35 (8)
O3^i—Cu1—N1	166.23 (9)	O3^i—Cu1—O5	95.77 (8)
O1—Cu1—N1	95.67 (8)	O1—Cu1—O5	98.81 (8)
O3^i—Cu1—N2	92.25 (9)	N1—Cu1—O5	96.28 (8)
O1—Cu1—N2	171.98 (8)	N2—Cu1—O5	88.93 (8)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O7—H7C$\cdots$O6	0.82 (6)	2.14 (7)	2.876 (5)	151 (10)
O7—H7B$\cdots$O2^{ii}	0.82 (6)	2.12 (6)	2.926 (4)	172 (10)
O5—H5B$\cdots$O2^{ii}	0.82	2.13	2.825 (3)	143
O5—H5C$\cdots$O4^i	0.82	2.03	2.691 (3)	137

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

H atoms attached to the C atoms were included in the refinement in calculated positions in the riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water H atoms were located and refined with distance restraints [O—H = 0.82 (1) Å and H···H = 1.39 (1) Å; $U_{iso}(H) = 1.2U_{eq}(O)$].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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