μ-Terephthalato-bis[aquachloro(1,10-phenanthroline)copper(II)]

Hong-Ping Xiao,* Xin-Hua Li, Ming-De Ye 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

Key indicators

Single-crystal X-ray study
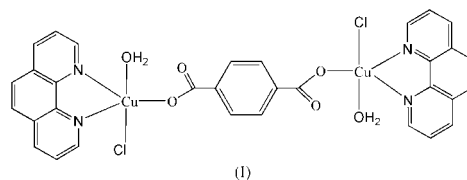$T = 273$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.076
Data-to-parameter ratio = 12.5

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

In the centrosymmetric title compound, $[Cu_2(C_8H_4O_4)Cl_2(C_{12}H_8N_2)_2(H_2O)_2]$, each Cu atom is surrounded by an O atom from a terephthalate dianion, a water molecule, a Cl atom and the N atoms from a 1,10-phenanthroline heterocycle in an octahedral arrangement. The terephthalate dianion, which functions as a bridge between two Cu atoms, lies on a special position of $\bar{1}$ site symmetry.

Comment

Among the metal complexes of terephthalic acid (Fun *et al.*, 1999; Li *et al.*, 1998; Mori & Takamizawa, 2000), the copper–phenanthroline (phen) system has been well studied; the compounds structurally documented include, for example, dimeric $[Cu_2(C_8H_4O_4)(phen)_4](ClO_4)_2$ and three polymeric complexes, *viz.* $[Cu(C_8H_4O_4)(phen)]$, $[Cu(C_8H_4O_4)(phen)(H_2O)]$ and $[Cu(C_8H_4O_4)(phen)(H_2O)](H_2O)(C_3H_7ON)$ (Sun *et al.*, 2000, 2001; Zhu *et al.*, 2004). In our previous work, we obtained a chain polymer with both terephthalate dianion and chloro bridges, *viz.* $[Cu_2Cl_2(nphen)_2(C_8H_4O_4)]\cdot 2C_3H_7ON$, where nphen is replaced by 5-nitro-1,10-phenanthroline (nphen) (Xiao & Zhu, 2003). In the present compound, (I), the Cu atom is linked to four different ligands.

(I)

In centrosymmetric (I), the Cu atom is surrounded by an O atom from a terephthalate dianion, a water molecule, a Cl atom and the N atoms from a 1,10-phenanthroline heterocycle in an octahedral arrangement. The terephthalate dianion, which functions as a bridge between two Cu atoms, lies on a special position of $\bar{1}$ site symmetry. The Cu1—O1 bond length [1.9455 (15) Å] is in agreement with analogous literature distances in copper complexes containing a bis-monodentate terephthalate ligand (Cano *et al.*, 1997; Deakin *et al.*, 1999; Li
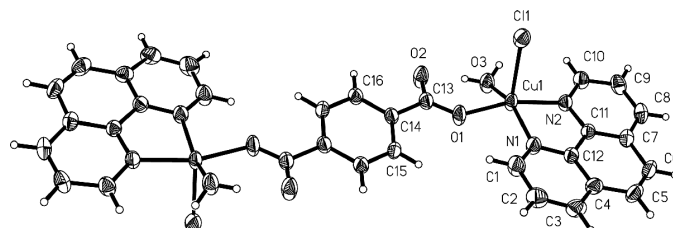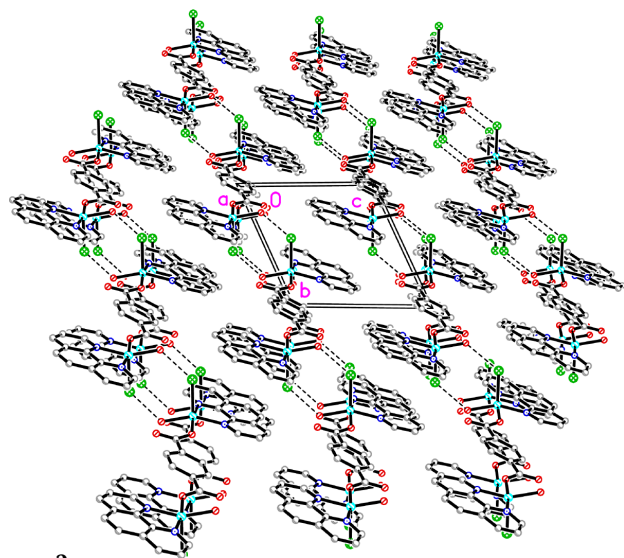

Figure 1
The structure of (I), with the atom numbering of the asymmetric unit, showing displacement ellipsoids at the 50% probability level.

Figure 2
Zigzag chains formed by hydrogen-bonding interactions, which are shown as dashed lines. H atoms have been omitted.

et al., 2001; Xanthopoulos *et al.*, 1993). The aromatic rings of the terephthalate and phen ligands are almostly coplanar, the dihedral angle being only 5.90 (6)°. The Cu···Cu distance [11.13 (6) Å] through the bridging terephthalate ligand is also in agreement with that reported for bis-monodentate terephthalate-bridged copper(II) complexes (Cano *et al.*, 1997; Sun *et al.*, 2000, 2001). There is one intramolecular hydrogen bond (O3—H3···O2) and also one intermolecular hydrogen bond [O3—H3B···Cl^i; symmetry code: (i) $1 - x$, $1 - y$, $-z$], resulting in the formation of zigzag chains (Fig. 2).

Experimental

A solution (10 ml) of dimethylformamide containing CoCl₂·6H₂O (0.5 mmol, 0.12 g), CuCl₂·2H₂O (0.5 mmol, 0.09 g) and terephthalic acid (0.5 mmol, 0.08 g) was added slowly to a solution (10 ml) of dimethylformamide containing 1,10-phenanthroline (0.5 mmol, 0.10 g). The mixture was stirred for 30 min and left to stand at room temperature for about a month, after which time green prismatic crystals were obtained.

Crystal data

[Cu₂(C₈H₄O₄)Cl₂(C₁₂H₈N₂)₂(H₂O)₂]	$Z = 1$
$M_r = 758.55$	$D_x = 1.710$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.6846$ (10) Å	Cell parameters from 678
$b = 9.7645$ (11) Å	reflections
$c = 10.4676$ (12) Å	$\theta = 2.4–22.0°$
$\alpha = 63.154$ (2)°	$\mu = 1.68$ mm^{-1}
$\beta = 68.579$ (2)°	$T = 273$ (2) K
$\gamma = 78.644$ (2)°	Prism, green
$V = 736.74$ (15) Å^3	$0.40 \times 0.31 \times 0.28$ mm

Data collection

Bruker SMART APEX area-detector diffractometer	2628 independent reflections
φ and ω scans	2458 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$R_{int} = 0.014$
$T_{min} = 0.545$, $T_{max} = 0.632$	$\theta_{max} = 25.2°$
5423 measured reflections	$h = -10 \rightarrow 10$
	$k = -11 \rightarrow 11$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.043P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$+ 0.2928P]$
$wR(F^2) = 0.076$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
2628 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
210 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXTL*
	Extinction coefficient: 0.0009 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.0267 (18)	Cu1—O3	1.9992 (15)
Cu1—N2	2.0187 (17)	Cu1—Cl1	2.4895 (7)
Cu1—O1	1.9455 (15)		
N1—Cu1—N2	81.46 (7)	N2—Cu1—O3	95.41 (7)
N1—Cu1—O1	87.57 (7)	N2—Cu1—Cl1	93.72 (5)
N1—Cu1—O3	152.70 (8)	O1—Cu1—O3	90.06 (7)
N1—Cu1—Cl1	105.83 (6)	O1—Cu1—Cl1	98.27 (6)
N2—Cu1—O1	165.59 (7)	O3—Cu1—Cl1	101.43 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	1.86	2.612 (2)	152
O3—H3B···Cl1^i	0.82	2.31	3.0743 (16)	155

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

The water H atoms were refined subject to the restraint O—H = 0.82 (1) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å and with $U_{iso} = 1.2U_{eq}$(parent atom).

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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