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μ-Terephthalato-bis[bis(2,2′-bipyridine)copper(II)] bis(perchlorate) dihydrate

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Key indicators

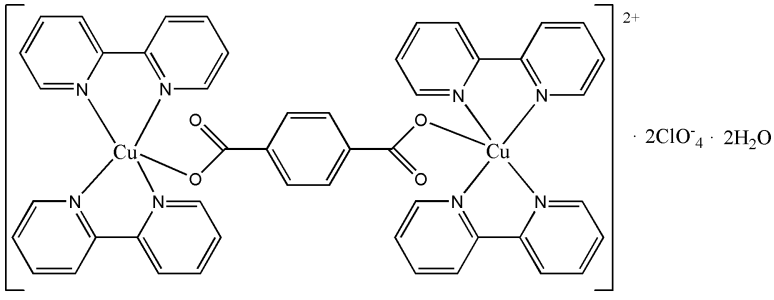
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.123
Data-to-parameter ratio = 12.2

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

In the title compound, $[Cu_2(C_8H_4O_4)(C_{10}H_8N_2)_4](ClO_4)_2\cdot 2H_2O$, each Cu atom is surrounded by an O atom of a terephthalate dianion and four N atoms of two 2,2′-bipyridine molecules, forming a distorted square-pyramidal geometry. The terephthalate dianion functions as a bridge between two Cu atoms and forms a dinuclear complex.

Comment

During the study of the structures of complexes in the Cu^{2+}/phen/H_2tp (phen is 1,10-phenanthroline and H_2tp is terephthalic acid) system (Cano *et al.*, 1997; Chen *et al.*, 2004; Sun *et al.*, 2000, 2001; Xiao *et al.*, 2004; Zhu *et al.*, 2004) and in the Cu^{2+}/2,2′-bipy/H_2tp (2,2′-bipy is 2,2′-bipyridine) system (Xiao & Zhu, 2003; Li & Xiao, 2004), we obtained a series of dinuclear complexes and one-dimensional zigzag chain coordination polymers. These complexes display a diversity of structures, and new complexes are constantly being produced through different reactions, and even by a small change in preparation conditions, such as the use of different solvents, temperature or H-atom acceptors. All of these factors encouraged us to research these systems more deeply. The title compound, (I), represents an example.



(I)

Each Cu atom is surrounded by an O atom of a terephthalate dianion and four N atoms of two 2,2′-bipyridine molecules in a distorted square-pyramidal geometry (Fig. 1 and Table 1). The 2,2′-bipyridine group acts as a chelating ligand and the terephthalate dianion functions as a bridge between two Cu atoms in a bis-monodentate coordination mode. However, the Cu1—O2 distance [2.803 (3) Å] suggests a weak interaction between the uncoordinated O atom and the Cu atom. Hence, the Cu atom may be also regarded as having a distorted octahedral geometry. The dinuclear cations, perchlorate anions and solvent water molecules interact through multimolecular interactions, generating a polymeric framework (Fig. 2).

Experimental

An aqueous solution (10 ml) of copper chloride dihydrate (0.3 mmol) was added dropwise to a solution (10 ml) of dimethylformamide containing 2,2′-bipyridine (0.3 mmol), terephthalic acid (0.3 mmol) and 2,2′-dithiosalicylic acid (0.3 mmol) at room temperature. The reaction mixture was filtered and the filtrate was left to stand for about four weeks until blue single crystals were obtained.

Crystal data

$[Cu(C_8H_4O_4)(C_{10}H_8N_2)_4](ClO_4)_2\cdot 2H_2O$
$M_r = 1150.86$
Triclinic, $P\overline{1}$
$a = 9.9505$ (14) Å
$b = 11.1049$ (14) Å
$c = 12.1187$ (14) Å
$\alpha = 74.621$ (2)°
$\beta = 66.750$ (2)°
$\gamma = 89.352$ (2)°
$V = 1179.7$ (3) Å^3
$Z = 1$
$D_x = 1.620$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4176 reflections
$\theta = 1.9$–25.2°
$\mu = 1.09$ mm^{-1}
$T = 298$ (2) K
Prism, blue
0.35 × 0.20 × 0.17 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.77$, $T_{max} = 0.83$
6347 measured reflections
4176 independent reflections
3707 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.2°$
$h = -11 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.123$
$S = 1.05$
4176 reflections
342 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2 + 0.902P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.990 (2)	Cu1—N1	2.038 (2)
Cu1—N2	1.998 (3)	Cu1—N4	2.203 (3)
Cu1—N3	2.008 (3)		
O1—Cu1—N2	92.12 (10)	N3—Cu1—N1	93.83 (10)
O1—Cu1—N3	92.74 (9)	O1—Cu1—N4	98.74 (9)
N2—Cu1—N3	174.70 (10)	N2—Cu1—N4	103.22 (10)
O1—Cu1—N1	163.82 (10)	N3—Cu1—N4	78.10 (10)
N2—Cu1—N1	80.93 (10)	N1—Cu1—N4	97.07 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O4^{i}	0.78 (4)	2.48 (4)	3.239 (8)	164 (5)
O7—H7A···O2^{ii}	0.77 (4)	2.21 (4)	2.916 (5)	153 (6)

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1+x, y, z$.

Water H atoms were refined subject to the restraint O—H = 0.82 (5) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å with $U_{iso} = 1.2U_{eq}$(C).

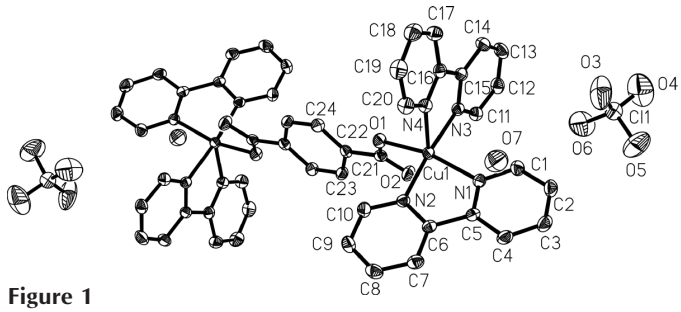


Figure 1
The structure of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity. Unlabelled atoms are related to labelled atoms by the symmetry code $(-x, -y, -z)$.

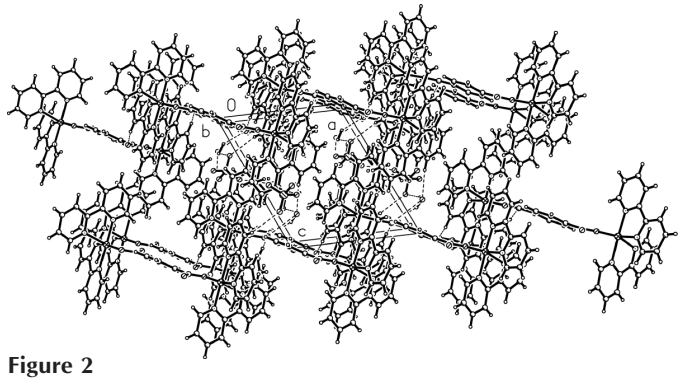


Figure 2
Perspective view, along the b axis, of the molecular packing of (I), assembled by multimolecular interactions (dashed lines).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000; data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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