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Bis[bis(1,10-phenanthroline)chlorocopper(II)] benzene-1,2,4,5-tetracarboxylate(2−) dihydrate

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

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

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

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In the title compound, $[CuCl(C_{12}H_8N_2)_2]_2(C_{10}H_4O_8)\cdot 2H_2O$, the Cu^{II} cation has a five-coordinate environment made up of one chloride anion and four N atoms of two 1,10-phenanthroline ligands. Hydrogen bonds between the benzene-1,2,4,5-tetracarboxylate(2−) anion and water molecules produce a linear hydrogen-bonded chain. The anion lies on a special position of $\overline{1}$ site symmetry.

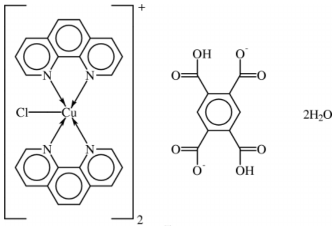
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.091
Data-to-parameter ratio = 11.7

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

Comment

The synthesis of new coordination polymers is of current interest in the field of crystal engineering and supramolecular chemistry owing to the crystal-packing motifs that give rise to potential properties as functional materials (Kitagawa & Kondo, 1998; Mori *et al.*, 2000; Song *et al.*, 2003). Multicarboxylate building blocks such as benzene-1,4-dicarboxylic acid (H_2BDC) and benzene-1,2,4,5-tetracarboxylatic acid (H_4TCB) can produce the desired networks in metal-organic polymers (Gutschke *et al.*, 2001; Lo *et al.*, 2000; Xiao & Zhu, 2003; Yang *et al.*, 2003). However, complexes made from H_4TCB, phen and Cu^{II} building blocks are rather limited (Hu *et al.*, 2003; Shi *et al.*, 2001), and the title complex, $[CuCl(phen)_2]_2(H_2TCB)\cdot 2H_2O$, (I), represents an example.



(I)

The coordination geometry of the Cu atom is best described as a distorted trigonal bipyramid made up of one chloride anion and four N atoms of two phen molecules (Fig. 1). The H_2TCB^{2-} anion is free and does not coordinate to the Cu atom, whereas in $[Cu(phen)(H_2TCB)]_n$, the H_2TCB^{2-} anion displays a μ_2-bridging mode (Hu *et al.*, 2003). In the $[CuCl(phen)_2]^+$ cation, two phen molecules are almost perpendicular to each other.

There are two types of hydrogen bonds: one intramolecular (O3—H32···O2) and two intermolecular [O5—H30···O1^{i} and O5—H31···O1^{ii}; symmetry codes: (i) $x-1$, y, z; (ii) $1-x$, $1-y$, $1-z$]. The free water molecules and H_2TCB^{2-} anions form a hydrogen-bonded chain. The distance between adjacent chains is 11.336 (8) Å, the b axis length. The $[CuCl(phen)_2]^+$ cations occupy the space between the chains and there are π–π stacking interactions of the phen rings,

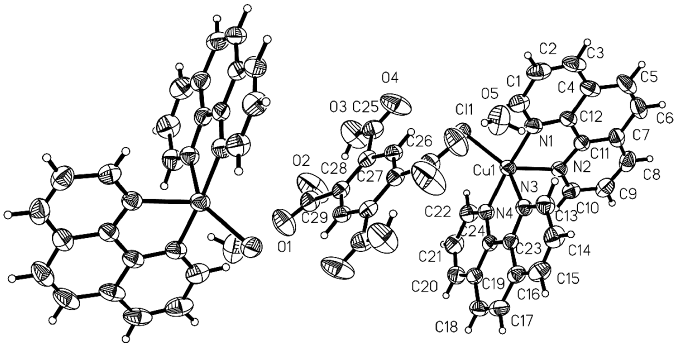


Figure 1
Twice the asymmetric unit of (I), with atom numbering, showing displacement ellipsoids at the 50% probability level.

between two neighboring cations, at a distance of approximately 3.66 Å.

Experimental

A solution (10 ml) of dimethylformamide containing $CuCl_2 \cdot 2H_2O$ (0.043 g, 0.25 mmol) and H_4TCB (0.13 g, 0.5 mmol) was added slowly to a solution (10 ml) of dimethylformamide containing 1,10-phenanthroline (0.10 g, 0.5 mmol). The mixture was left to stand at room temperature for about two weeks to afford green prisms.

Crystal data

$[CuCl(C_{12}H_8N_2)_2]_2(C_{10}H_4O_8) \cdot 2H_2O$
$M_r = 1206.96$
Triclinic, $P\overline{1}$
$a = 10.1324\ (7)$ Å
$b = 11.3356\ (8)$ Å
$c = 12.2000\ (9)$ Å
$\alpha = 104.0410\ (10)°$
$\beta = 95.2080\ (10)°$
$\gamma = 110.6850\ (10)°$
$V = 1247.48\ (15)$ Å^3
$Z = 1$
$D_x = 1.607$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 426 reflections
$\theta = 2.3$–$21.4°$
$\mu = 1.03$ mm^{-1}
$T = 273\ (2)$ K
Prism, green
0.34 × 0.28 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.714$, $T_{max} = 0.874$
6633 measured reflections
4388 independent reflections
3992 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.1°$
$h = -11 \rightarrow 12$
$k = -13 \rightarrow 8$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.091$
$S = 1.07$
4388 reflections
374 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.4259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0094 (12)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.9949 (18)	Cu1—N4	2.0047 (18)
Cu1—N2	2.1569 (18)	Cu1—Cl1	2.2763 (6)
Cu1—N3	2.1071 (17)		
N1—Cu1—N2	80.38 (7)	N2—Cu1—N3	93.90 (7)
N1—Cu1—N3	94.34 (7)	N2—Cu1—Cl1	121.04 (5)
N1—Cu1—N4	174.67 (7)	N3—Cu1—N4	80.70 (7)
N1—Cu1—Cl1	92.15 (5)	N3—Cu1—Cl1	145.05 (5)
N2—Cu1—N4	97.93 (7)	N4—Cu1—Cl1	93.04 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H31···O1^{ii}	0.855 (10)	2.025 (14)	2.864 (3)	167 (3)
O5—H30···O1^{i}	0.849 (10)	2.313 (17)	3.096 (3)	154 (3)
O3—H32···O2	0.851 (10)	1.593 (18)	2.404 (3)	158 (4)

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

H atoms bonded to O were refined subject to the restraint O—H = 0.85 (2) 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).

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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