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Chlorobis(1,10-phenanthroline)copper(II) 5-nitroisophthalate(1–) dihydrate

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In the title compound, $[CuCl(C_{12}H_8N_2)_2](C_8H_4NO_6)\cdot 2H_2O$, the coordination geometry of the Cu atom is best described as distorted trigonal bipyramidal, made up of four N atoms of two phenanthroline molecules and one chloride anion. The 5-nitroisophthalate(1−) anion is uncomplexed and balances the charge. π–π stacking and intermolecular hydrogen-bond interactions link the components units into a three-dimensional network structure.

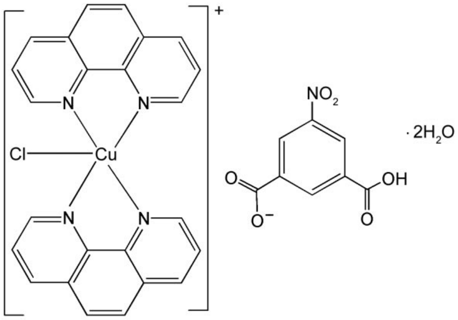
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.013 Å
R factor = 0.103
wR factor = 0.204
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.

Comment

The development of metal-organic supramolecular architectures is a rapidly developing area of research, not only because of their intriguing structural motifs but also in view of their potential applications in host–guest chemistry (Feng & Xu, 2001; Leininger & Olenyuk, 2000). In this field, aromatic polycarboxylic acids such as benzene-1,2,4,5-tetracarboxylic acid, benzene-1,4-dicarboxylic acid, isophthalic acid and their derivates have been extensively used (Si *et al.*, 2004; Xiao *et al.*, 2004; Zhu *et al.*, 2004). We investigate here the effect of replacing isophthalic acid with 5-nitroisophthalic acid. In a mixed solution of dimethylformamide and methanol at room temperature, we obtained the title compound, (I).



(I)

Compound (I) consists of a $[CuCl(phen)_2]^+$ cation (phen = 1,10-phenanthroline), a 5-nitroisophthalate(1−) anion and two uncoordinated water molecules. The coordination geometry of the Cu atom is best described as distorted trigonal bipyramidal, made up of four N atoms of two 1,10-phenanthroline molecules and one chloride anion (Fig. 1 and Table 1). The 5-nitroisophthalate(1−) counter-anion is free and does not coordinate to the Cu atom. In the $[CuCl(phen)_2]^+$ cation, the dihedral angle between the two phen ligand planes is 70.50 (2)°.

The short interplanar distance of 3.52 Å between the 1,10-phenanthroline and benzene rings of the 5-nitroisophthalate(1−) anion from neighboring units indicates on the existence of π–π stacking. Intermolecular O—H···Cl and

O—H···O hydrogen bonds (Table 2) are also found in the crystal structure. All these interactions link the various components into a three-dimensional network structure (Fig. 2).

Experimental

A solution (15 ml) of dimethylformamide containing $CuCl_2·2H_2O$ (0.5 mmol, 0.852 g) and 5-nitroisophthalic acid (0.5 mmol, 0.105 g) was added slowly to a solution (5 ml) of methanol containing 1,10-phenanthroline (0.5 mmol, 0991 g). The mixture was left to stand at room temperature for about two weeks, affording blue crystals.

Crystal data

$[CuCl(C_{12}H_8N_2)_2](C_8H_4NO_6)·2H_2O$
$M_r = 705.55$
Triclinic, $P\overline{1}$
$a = 10.5099 (13)$ Å
$b = 12.1597 (14)$ Å
$c = 12.5348 (14)$ Å
$\alpha = 72.798 (3)°$
$\beta = 84.990 (2)°$
$\gamma = 77.968 (3)°$
$V = 1496.1 (3)$ Å^3

$Z = 2$
$D_x = 1.566$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 476 reflections
$\theta = 2.6–24.1°$
$\mu = 0.88$ mm^{-1}
$T = 298 (2)$ K
Rod, blue
0.13 × 0.06 × 0.05 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: by multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.894$, $T_{max} = 0.957$
11046 measured reflections

5344 independent reflections
3112 reflections with $I > 2\sigma(I)$
$R_{int} = 0.097$
$\theta_{max} = 25.2°$
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.103$
$wR(F^2) = 0.204$
$S = 1.08$
5344 reflections
437 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.4686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.002 (6)	Cu1—N3	2.168 (7)
Cu1—N4	2.002 (6)	Cu1—Cl1	2.287 (2)
Cu1—N2	2.082 (6)		
N1—Cu1—N4	174.6 (3)	N2—Cu1—N3	108.1 (2)
N1—Cu1—N2	81.0 (3)	N1—Cu1—Cl1	94.8 (2)
N4—Cu1—N2	97.1 (2)	N4—Cu1—Cl1	89.93 (19)
N1—Cu1—N3	96.3 (2)	N2—Cu1—Cl1	139.31 (19)
N4—Cu1—N3	79.4 (2)	N3—Cu1—Cl1	112.61 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8B···Cl1^{i}	0.82 (6)	2.64 (4)	3.420 (10)	160 (8)
O8—H8A···O1	0.83 (7)	1.90 (5)	2.642 (10)	149 (8)
O7—H7B···O8^{ii}	0.80 (3)	1.95 (3)	2.718 (11)	163 (7)
O7—H7A···O3^{iii}	0.80 (5)	1.73 (6)	2.526 (8)	176 (8)
O2—H2A···O7^{i}	0.82	1.94	2.651 (9)	145

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

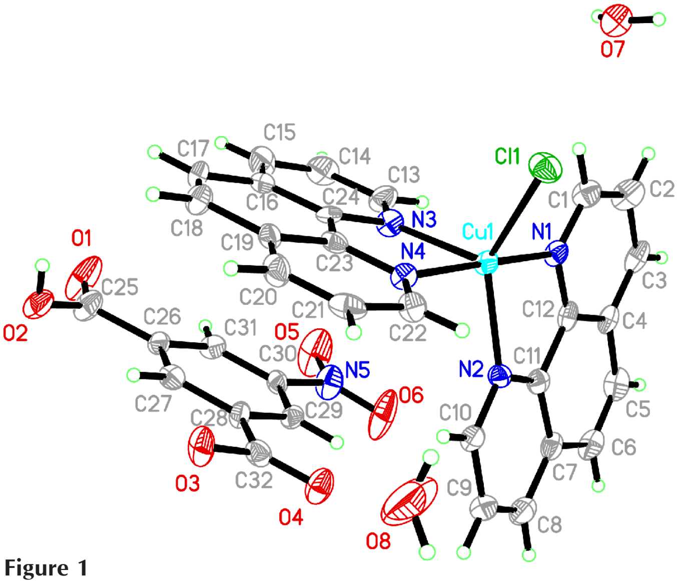


Figure 1
The asymmetric unit of (I) with the atom numbering, showing displacement ellipsoids at the 50% probability level.

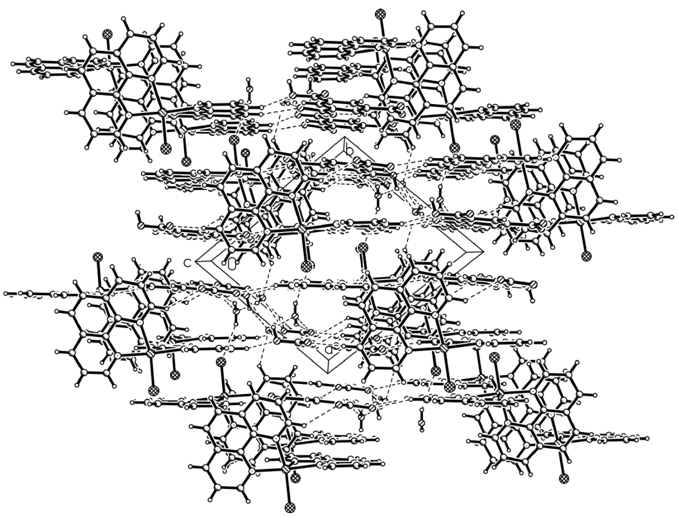


Figure 2
The crystal packing of (I). Hydrogen bonds are indicated by dashed lines.

H atoms attached to C atoms were included in the refinement in calculated positions in the riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. Water H atoms were located in a difference Fourier map and refined with distance restraints [O—H = 0.82 (2) Å and H···H = 1.45 (1) Å] and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2002)

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