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Chlorobis(1,10-phenanthroline)copper(II) 2-carboxybenzenesulfonate monohydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.054
wR factor = 0.127
Data-to-parameter ratio = 13.3

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

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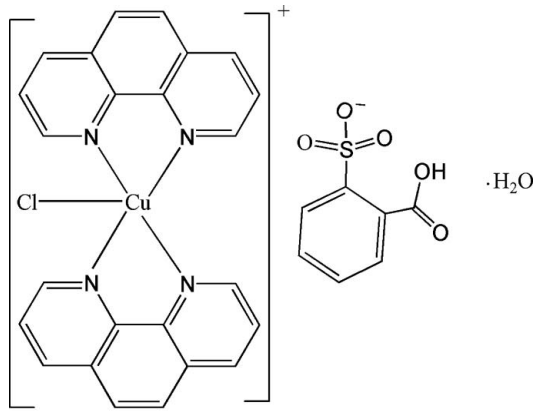
In the title compound, $[CuCl(C_{12}H_8N_2)_2](C_7H_5O_5S)\cdot H_2O$, copper(II) is coordinated by four N atoms and one chloride anion in a distorted trigonal-bipyramidal geometry. The Cu—N bond lengths are in the range 1.992 (3)–2.121 (3) Å, while the Cu—Cl distance is 2.3046 (11) Å.

Comment

In continuation of our study of the chemistry of carboxybenzenesulfonate ligands (Fan *et al.*, 2004; Li & Yang, 2004; Xiao, 2005; Xiao, Li & Hu, 2005; Xiao, Shi & Cheng, 2005; Zhang *et al.*, 2005), we present here the crystal structure of the title compound, $[CuCl(phen)_2](o\text{-sb})\cdot H_2O$ (phen is 1,10-phenanthroline; *o*-sb is 2-carboxybenzenesulfonate).



(I)

The title compound, (I), consists of a $[CuCl(phen)_2]^+$ cation, a 2-carboxybenzenesulfonate anion and one water molecules (Fig. 1). 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. The Cu—N bond lengths are in the range 1.992 (3)–2.121 (3) Å, while the Cu—Cl bond distance is 2.3046 (11) Å (Table 1). The 2-carboxybenzenesulfonate anion does not coordinate to the Cu atom, but simply balances the charge. The dihedral angle between the two phen ligands in (I) [59.60 (1)°] is much smaller than that [70.50 (2)°] observed in $[CuCl(phen)_2](C_7H_4NO_6)\cdot 2H_2O$ (Ye *et al.*, 2004).

The relatively short interplanar distances of 3.662 (2) Å between the 1,10-phenanthroline ring systems of neighbouring cations indicate a possible weak π–π stacking interaction. Intermolecular O—H···O hydrogen bonds (Table 2) link two 2-carboxybenzenesulfonate anions and two water molecules into a cluster. The crystal packing (Fig. 2) is additionally stabilized by van der Waals forces.

Experimental

An aqueous solution (15 ml) of $CuCl_2{\cdot}2H_2O$ (0.5 mmol, 0.852 g) was added slowly to a mixed solution (10 ml) of ethanol containing 1,10-phenanthroline (0.5 mmol, 0991 g) and 2-sulfobenzoic acid (0.5 mmol, 0.101 g). The mixture was left to stand at room temperature for about two weeks to afford green crystals.

Crystal data

$[CuCl(C_{12}H_8N_2)_2](C_7H_5O_5S){\cdot}H_2O$
M_r = 678.58
Triclinic, $P\overline{1}$
a = 8.0807 (10) Å
b = 13.2419 (16) Å
c = 14.5790 (18) Å
α = 68.321 (2)°
β = 83.256 (2)°
γ = 78.163 (2)°
V = 1417.4 (3) Å^3
Z = 2
D_x = 1.590 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3297 reflections
θ = 2.6–25.1°
μ = 0.99 mm^{-1}
T = 298 (2) K
Prism, green
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.811, T_{max} = 0.857
10971 measured reflections
5393 independent reflections
4715 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.8°
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.127
S = 1.12
5393 reflections
404 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.3918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.992 (3)	Cu1—N1	2.121 (3)
Cu1—N2	1.994 (3)	Cu1—Cl1	2.3046 (11)
Cu1—N4	2.103 (3)		
N3—Cu1—N2	174.43 (12)	N4—Cu1—N1	115.55 (11)
N3—Cu1—N4	80.79 (11)	N3—Cu1—Cl1	92.81 (9)
N2—Cu1—N4	96.36 (12)	N2—Cu1—Cl1	92.74 (9)
N3—Cu1—N1	96.22 (11)	N4—Cu1—Cl1	124.40 (8)
N2—Cu1—N1	80.63 (11)	N1—Cu1—Cl1	120.04 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.82	1.90	2.684 (3)	161
O6—H6A···O5^{ii}	0.87 (2)	2.00 (3)	2.823 (4)	156 (4)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-1, y, z+1$.

The water H atoms were located and refined with distance restraints [O—H = 0.85 (2) Å and U_{iso}(H) = 1.5U_{eq}(O)]. All other H atoms were included in the refinement in calculated positions in the riding-model approximation, with C–H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C), and O–H = 0.82 Å, U_{iso}(H) = 1.5U_{eq}(O).

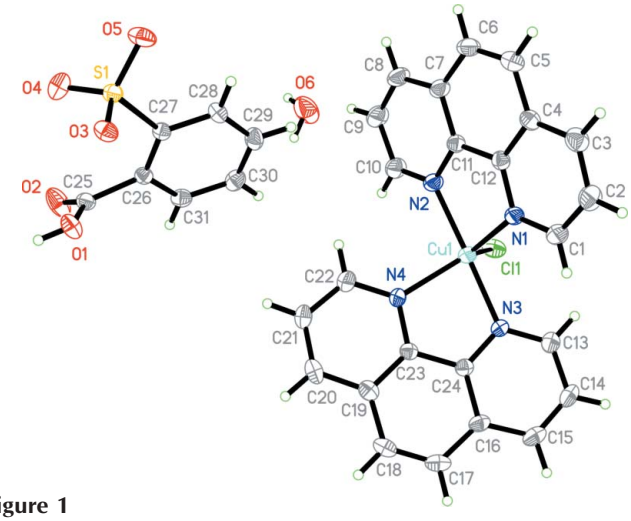


Figure 1
View of (I), showing the atom numbering and displacement ellipsoids at the 30% probability level.

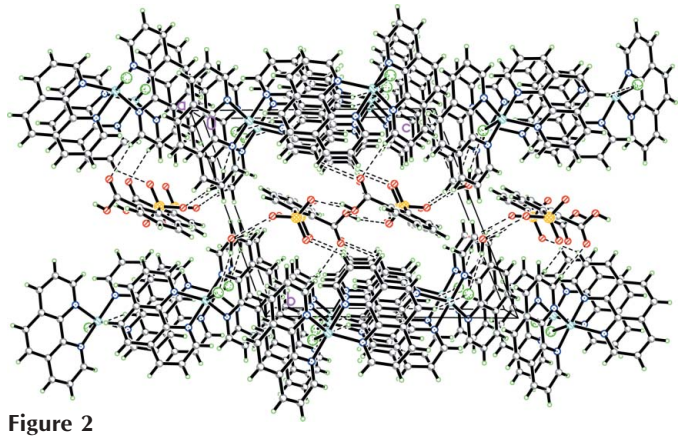


Figure 2
Crystal packing, viewed approximately along the *a* axis. The intermolecular hydrogen bonds are shown by dashed lines.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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