metal-organic papers

# Bis(2,2'-bipyridine-$\kappa^2 N,N'$)chlorocopper(II) 3-carboxybenzenesulfonate trihydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
H-atom completeness 93%
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.130
Data-to-parameter ratio = 12.8

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

In the title compound, $[CuCl(C_{10}H_8N_2)_2](C_7H_5O_5S)\cdot 3H_2O$, the Cu^{II} ion is coordinated by two 2,2-bipyridine and one chloro ligand in a trigonal–bipyramidal geometry. A hydrogen-bonding network consolidates the crystal structure.

Comment

Recently, we have studied metal complexes incorporating the carboxybenzenesulfonate (cbs) anion (Fan, Xiao, Zhang, Cai & Zhu, 2004; Fan, Xiao, Zhang & Zhu, 2004; Zhang *et al.*, 2005). As part of our ongoing investigation on the coordination properties of cbs, we present here the structure of the title compound, (I).
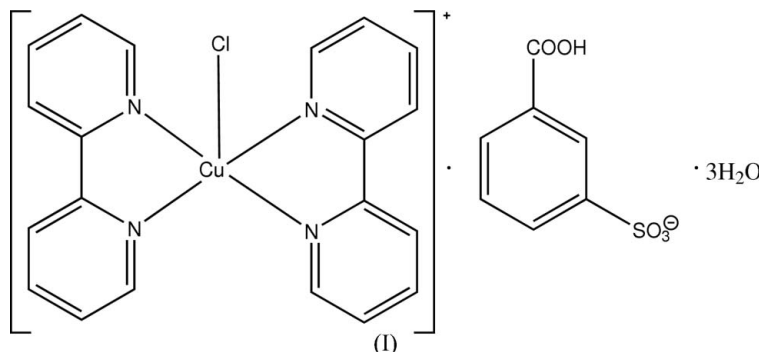
The crystal structure of (I) consists of $[CuCl(bipy)_2]^+$ cations (bipy is 2,2'-bipyridine), cbs anions and coordinated water molecules. In the cation, the Cu^{II} ion adopts a distorted trigonal–bipyramidal geometry defined by two bipy and one chloro ligand, with atoms N2 and N4 at the axial positions (Fig. 1 and Table 1). The axial Cu—N bond lengths are significantly shorter than those in the equatorial coordination plane. The Cu1—Cl1 bond length in (I) is comparable with those found in reported $[CuCl(bipy)_2]^+$ cations (Brandon *et al.*, 1995; Brophy *et al.*, 1999; O'Sullivan *et al.*, 1999). The Cu^{II} ion is essentially in the equatorial plane [the deviation being 0.014 (1) Å].

The cbs exists in (I) as a monoanion; the carboxyl group of cbs is not deprotonated and it does not coordinate to the metal ion. The sulfonate O atoms are hydrogen bonded to uncoordinated water molecules or bipy ligands of neighbouring complex cations (Table 2) to consolidate the crystal structure. No hydrogen bonding is observed between cation and anion in (I), but the partial overlapped arrangement and short centroid separation of 3.705 (2) Å suggest the existence of π–π stacking between benzene and pyridine rings.
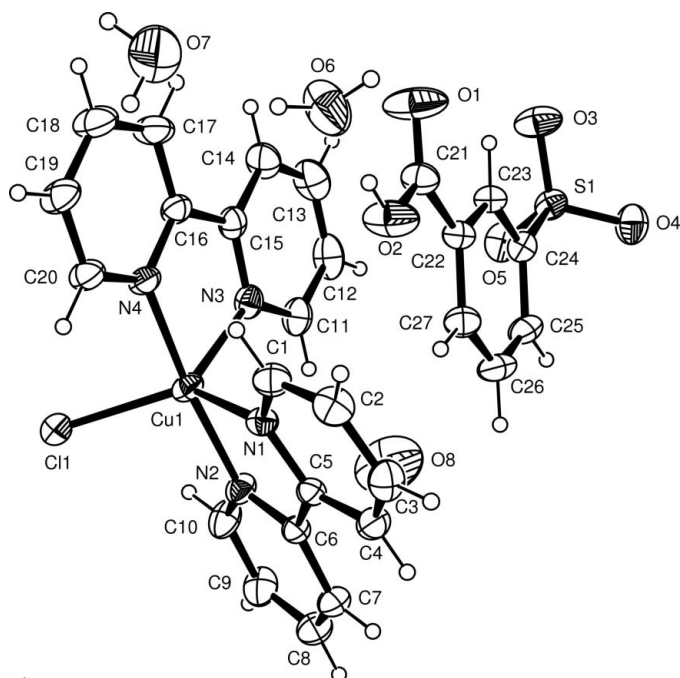
Figure 1
The molecular structure of (I), shown with 40% probability displacement ellipsoids (arbitrary spheres for H atoms). The minor occupancy component of the disordered water oxygen (O8′) has been omitted for clarity.

Experimental

A mixture of $CuCl_2 \cdot 2H_2O$ (0.170 g, 1 mmol), sodium 3-carboxybenzenesulfonate (0.224 g, 1 mmol), 2,2′-bipyridine (0.156 g, 1 mmol) and water (15 ml) was sealed in a 30 ml Teflon-lined stainless steel autoclave and heated at 423 K for 48 h. After cooling to room temperature, the solution was allowed to evaporate. After 2 d, blue crystals of (I) were obtained.

Crystal data

$[CuCl(C_{10}H_8N_2)_2](C_7H_5O_5S) \cdot 3H_2O$	$Z = 2$
$M_r = 666.58$	$D_x = 1.541$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.4430$ (5) Å	Cell parameters from 3862
$b = 11.2269$ (7) Å	reflections
$c = 15.8025$ (10) Å	$\theta = 2.6$–27.5°
$\alpha = 99.098$ (1)°	$\mu = 0.98$ mm^{-1}
$\beta = 91.778$ (1)°	$T = 295$ (2) K
$\gamma = 103.189$ (1)°	Block, blue
$V = 1436.53$ (15) Å^3	$0.38 \times 0.26 \times 0.24$ mm

Data collection

Bruker APEX area-detector diffractometer	4978 independent reflections
φ and ω scans	4525 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.014$
	$\theta_{max} = 25.0°$
$T_{min} = 0.707$, $T_{max} = 0.798$	$h = -10 \rightarrow 10$
7532 measured reflections	$k = -13 \rightarrow 13$
	$l = -18 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$+ 1.4378P]$
$wR(F^2) = 0.130$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
4978 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
389 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.084 (3)	Cu1—Cl1	2.3116 (10)
Cu1—N2	1.985 (3)	S1—O3	1.444 (3)
Cu1—N3	2.104 (3)	S1—O4	1.447 (3)
Cu1—N4	1.970 (3)	S1—O5	1.450 (3)
N1—Cu1—Cl1	130.39 (8)	N2—Cu1—N3	98.31 (12)
N2—Cu1—Cl1	93.41 (9)	N4—Cu1—N2	173.78 (12)
N3—Cu1—Cl1	118.41 (8)	N4—Cu1—N3	79.93 (11)
N4—Cu1—Cl1	92.67 (9)	O3—S1—O4	113.1 (2)
N2—Cu1—N1	80.22 (11)	O3—S1—O5	113.8 (2)
N1—Cu1—N3	111.19 (11)	O4—S1—O5	111.53 (18)
N4—Cu1—N1	94.80 (11)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O6—H6$A\cdots$O7	0.84	1.95	2.723 (6)	153
O6—H6$B\cdots$O4^i	0.84	2.00	2.801 (5)	158
O7—H7$A\cdots$O3^{ii}	0.87	2.17	3.022 (6)	165
O7—H7$B\cdots$O3^{iii}	0.88	2.21	3.071 (6)	164
O2—H2$A\cdots$O6	0.88	1.74	2.624 (5)	173
C3—H3$\cdots$O5^{iv}	0.93	2.43	3.358 (5)	173
C8—H8$\cdots$O5^v	0.93	2.45	3.379 (5)	177

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

H atoms on C atoms were placed in idealized positions and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms on O atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with U_{iso}(H) = 0.08 Å^2. The water molecule (O8) is disordered over two positions with an occupancy ratio of 0.67 (3):0.33 (3); the H atoms of the disordered water molecule were not located.

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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