

Zhao-Di Liu,<sup>a</sup> Min-Yu Tan<sup>b</sup> and  
Hai-Liang Zhu<sup>a\*</sup><sup>a</sup>Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, and <sup>b</sup>Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of ChinaCorrespondence e-mail:  
hailiang\_zhu@163.com

## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(C-C) = 0.009$  Å  
 $R$  factor = 0.057  
 $wR$  factor = 0.181  
Data-to-parameter ratio = 15.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Diaquabis(ethylenediamine- $\kappa^2N,N'$ )copper(II)  
bis(4-fluorobenzoate)

The title compound,  $[\text{Cu}(\text{C}_2\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2](\text{C}_7\text{H}_4\text{FO}_2)_2$ , is a mononuclear complex. The  $\text{Cu}^{\text{II}}$  atom, which lies on a crystallographic inversion centre, is coordinated by four N atoms from two ethylenediamine ligands and two O atoms from two water molecules, to form a slightly distorted octahedral geometry. All the N atoms of the ethylenediamine ligands, and all the O atoms in the water molecules and 4-fluorobenzoate anions, contribute to the formation of a hydrogen-bonded three-dimensional network.

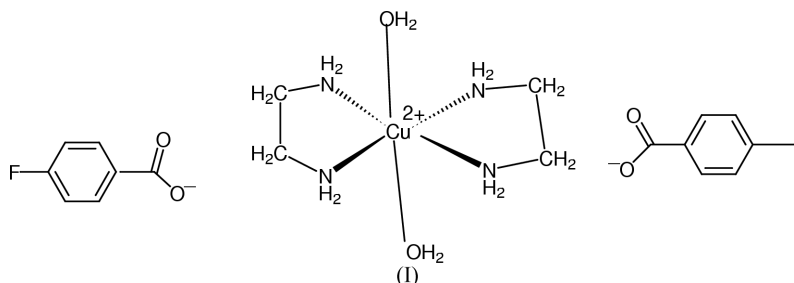
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## Comment

Amine complexes with transition metal carboxylates represent an important branch in the field of coordination chemistry. Previously, we have reported the crystal structures of some of these complexes (Zhu *et al.*, 1998, 1999, 2001, 2002; Zhu, Shao *et al.*, 2003; Zhu, Liu & Liu, 2003). As an extension of this work, we report here the title copper(II) complex, (I).



The asymmetric unit of (I) consists of one-half of the  $[\text{Cu}(\text{C}_2\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]^{2+}$  complex cation and an organic anion. The other half of the cation is generated by a crystallographic inversion centre. The  $\text{Cu}^{\text{II}}$  atom, which lies on the inversion centre, has a slightly distorted octahedral geometry. Two water molecules coordinate to the  $\text{Cu}^{\text{II}}$  atom in the axial positions, while four amino N atoms from two ethylenediamine ligands occupy the equatorial positions (Fig. 1). The  $\text{Cu}-\text{N}$  distances of 2.018 (4) and 2.021 (4) Å show normal values. In similar complexes, the  $\text{Cu}-\text{N}$  bond lengths lie in the range 2.00–2.05 Å (Li *et al.*, 1999; Procter *et al.*, 1968). The  $\text{Cu}-\text{O}_{\text{water}}$  distance of 2.579 (4) Å is appreciably longer than for other copper(II) complexes with water (Amirov *et al.*, 2003).

$\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Fig. 2) link the complex cations and anions of (I) into a three-dimensional network.

Experimental

A solution of  $\text{NH}_2(\text{CH}_2)_2\text{NH}_2 \cdot \text{H}_2\text{O}$  (1:5,  $v/v$ , 10 ml) containing copper(II) 4-fluorobenzoate tetrahydrate (1 mmol, 0.34 g) was stirred for 30 min in air, and then placed in a Parr Teflon-lined stainless steel vessel (18 ml). The vessel was sealed and heated at 433 K for 12 h, cooled to 373 K at a rate of 8 K  $\text{h}^{-1}$ , held at that temperature for 10 h and then cooled to room temperature to obtain violet crystals of (I). The crystals were isolated, washed with water and dried *in vacuo* using  $\text{CaCl}_2$  (yield 56.6%). Analysis found: C 43.39, H 5.74, N 11.30, O 19.34, F, 7.56%; calculated for  $\text{C}_{18}\text{H}_{28}\text{CuF}_2\text{N}_4\text{O}_6$ : C 43.41, H 5.67, N 11.25, O 19.28, F 7.63%.

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2](\text{C}_7\text{H}_4\text{FO}_2)_2$   $Z = 1$   
 $M_r = 497.98$   $D_x = 1.467 \text{ Mg m}^{-3}$   
 Triclinic,  $P\bar{1}$  Mo  $K\alpha$  radiation  
 Cell parameters from 2238 reflections  
 $a = 6.131(1) \text{ \AA}$   $\theta = 6\text{--}28^\circ$   
 $b = 7.144(1) \text{ \AA}$   $\mu = 1.03 \text{ mm}^{-1}$   
 $c = 14.498(3) \text{ \AA}$   $T = 293(2) \text{ K}$   
 $\alpha = 95.72(3)^\circ$  Block, violet  
 $\beta = 96.37(3)^\circ$   $0.30 \times 0.20 \times 0.10 \text{ mm}$   
 $\gamma = 115.15(3)^\circ$   
 $V = 563.6(2) \text{ \AA}^3$

Data collection

Siemens SMART CCD area-detector diffractometer 2238 independent reflections  
 2167 reflections with  $I > 2\sigma(I)$   
 $\varphi$  and  $\omega$  scans  $R_{\text{int}} = 0.019$   
 Absorption correction: multi-scan  $\theta_{\text{max}} = 26.5^\circ$   
 (*SADABS*; Sheldrick, 1996)  $h = -7 \rightarrow 7$   
 $T_{\text{min}} = 0.748$ ,  $T_{\text{max}} = 0.904$   $k = -8 \rightarrow 8$   
 4314 measured reflections  $l = -18 \rightarrow 18$

Refinement

Refinement on  $F^2$   $w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 1.8621P]$   
 $R[F^2 > 2\sigma(F^2)] = 0.057$  where  $P = (F_o^2 + 2F_c^2)/3$   
 $wR(F^2) = 0.181$   $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $S = 1.18$   $\Delta\rho_{\text{max}} = 1.74 \text{ e \AA}^{-3}$   
 2238 reflections  $\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$   
 148 parameters  
 H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu1—N1	2.018 (4)	Cu1—O1W	2.579 (4)
Cu1—N2	2.021 (4)		
N1 <sup>i</sup> —Cu1—N1	180	N1 <sup>i</sup> —Cu1—O1W	87.24 (14)
N1 <sup>i</sup> —Cu1—N2	84.95 (17)	N1—Cu1—O1W	92.76 (14)
N1—Cu1—N2	95.05 (17)	N2—Cu1—O1W	91.01 (15)
N2—Cu1—N2 <sup>i</sup>	180	N2 <sup>i</sup> —Cu1—O1W	88.99 (15)

Symmetry code: (i)  $-x, -y, -z$ .

Table 2

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N1 <sup>i</sup> —H1B <sup>ii</sup> ···O1	0.90	2.18	3.049 (6)	161
N1—H1D···O1W <sup>i</sup>	0.90	2.17	3.057 (6)	169
N2—H2C···O1 <sup>iii</sup>	0.90	2.29	3.079 (6)	147
N2—H2D···O2 <sup>iii</sup>	0.90	2.13	2.990 (6)	161
O1W—H1WA···O1 <sup>iii</sup>	0.837 (10)	1.936 (15)	2.766 (5)	171 (6)
O1W—H1WB···O2	0.836 (10)	1.973 (19)	2.778 (5)	161 (5)

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

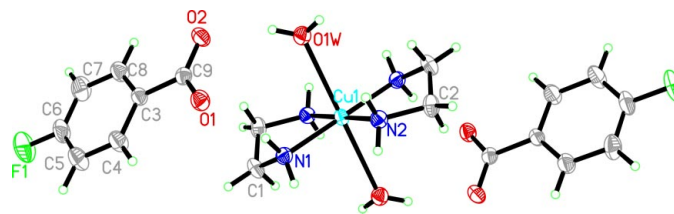


Figure 1 The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme for the contents of the asymmetric unit.

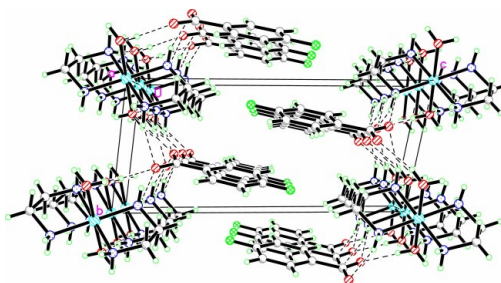


Figure 2 The crystal packing of (I), with the N—H···N and O—H···N hydrogen-bonding interactions shown as dashed lines.

The H atoms of the water molecules were located in a difference Fourier map and refined isotropically, with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2)  $\text{\AA}$ , respectively. The other H atoms were placed in geometrically idealized positions, with N—H = 0.90  $\text{\AA}$  and C—H = 0.96  $\text{\AA}$ , and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 0.08 \text{ \AA}^2$ . A large residual peak of 1.74 and 1.85  $\text{e \AA}^{-3}$  was observed 1.74 and 1.85  $\text{\AA}$  from atoms Cu1 and N1, respectively, but it does not make sense chemically or geometrically. Some minor non-merohedral twinning is observed as there is a consistent trend with  $F_o^2 \gg F_c^2$ , but we were unable to establish the twin law.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINTE* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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