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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
 $R$  factor = 0.057  
 $wR$  factor = 0.168  
Data-to-parameter ratio = 12.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.A mononuclear copper(II) compound derived  
from *N*-(2-hydroxyethyl)ethylenediamine

The asymmetric unit of the title compound bis[*N*-(2-hydroxyethyl)ethylenediamine- $\kappa^3N,N',O$ ]copper(II) bis(4-fluorobenzoate),  $[\text{Cu}(\text{C}_4\text{H}_{12}\text{N}_2\text{O})_2](\text{C}_7\text{H}_4\text{FO}_2)_2$ , contains one-half of a  $[\text{Cu}(\text{C}_4\text{H}_{12}\text{N}_2\text{O})_2]^{2+}$  complex cation (the other half is inversion-related) and a 4-fluorobenzoate anion. The  $\text{Cu}^{\text{II}}$  atom has a distorted octahedral coordination geometry and is surrounded by four N atoms and two O atoms from the two inversion-related *N*-(2-hydroxyethyl)ethylenediamine ligands. In the crystal structure, the molecules are held together by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, leading to the formation of a three-dimensional network.

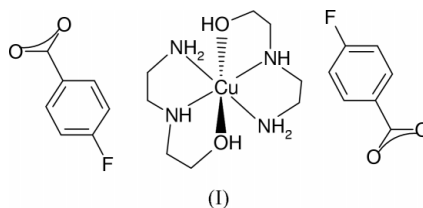
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## Comment

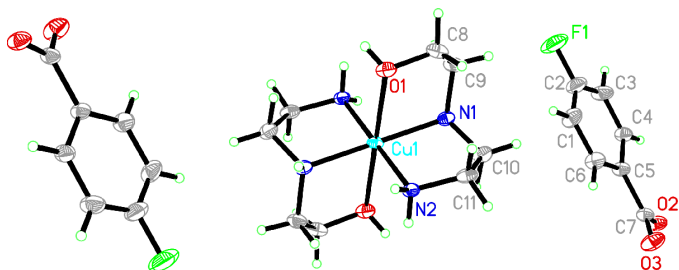
Metal-ethanolamine complexes are among the most investigated compounds in coordination chemistry. As an extension of the work, we report here the crystal structure of the title compound, (I), a  $\text{Cu}^{\text{II}}$  complex incorporating the ligand *N*-(2-hydroxyethyl)ethylenediamine.



The asymmetric unit of (I) contains one-half of a  $[\text{Cu}(\text{C}_4\text{H}_{12}\text{N}_2\text{O})_2]^{2+}$  complex cation and an uncoordinated 4-fluorobenzoate anion (Fig. 1). 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 and is coordinated by four N atoms and two O atoms from two *N*-(2-hydroxyethyl)ethylenediamine ligands. The two O atoms coordinate to the  $\text{Cu}^{\text{II}}$  atom in *trans* positions, while the four N atoms occupy the equatorial positions. The three *trans* angles at the  $\text{Cu}^{\text{II}}$  atom are  $180^\circ$  by symmetry (Table 1) and the other angles subtended at the  $\text{Cu}^{\text{II}}$  atom are close to  $90^\circ$ , varying from  $78.22(15)$  to  $101.78(15)^\circ$ , indicating a slightly distorted octahedral geometry. The average  $\text{Cu}-\text{N}$  bond length [ $2.024(4)$  Å] is comparable to that observed in a similar compound [ $2.045(8)$  Å; Vinogradova *et al.*, 2003].

In the 4-fluorobenzoate anion, the carboxylate group is twisted away from the plane of the benzene ring. The dihedral angle between the planes of the benzene ring and carboxylate group is  $18.0(7)^\circ$ .

In the crystal structure, all of the O atoms and N atoms contribute to the formation of hydrogen bonds, leading to the formation of a three-dimensional network (Fig. 2 and Table 2).



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

## Experimental

All reagents and solvents were used as obtained without further purification. Cupric 4-fluorobenzoate (0.5 mmol, 170.1 mg) and *N*-(2-hydroxyethyl)ethylenediamine (1.0 mmol, 102.2 mg) were dissolved in ethanol (50 ml). The mixture was stirred for 1 h to give a clear blue solution. After keeping the solution in air for two weeks, large blue block-shaped crystals had formed at the bottom of the vessel. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using  $P_4O_{10}$  (yield 45.7%). Analysis found: C 47.7, H 6.1, N 10.3%; calculated for  $C_{22}H_{32}CuF_2N_4O_6$ : C 48.0, H 5.9, N 10.2%.

### Crystal data

$[Cu(C_4H_4F_2O_2)_2](C_7H_4FO_2)_2$	$Z = 1$
$M_r = 550.06$	$D_x = 1.538 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.094(2) \text{ \AA}$	Cell parameters from 1012 reflections
$b = 7.353(2) \text{ \AA}$	$\theta = 2.5\text{--}19.7^\circ$
$c = 12.139(2) \text{ \AA}$	$\mu = 0.98 \text{ mm}^{-1}$
$\alpha = 102.68(3)^\circ$	$T = 293(2) \text{ K}$
$\beta = 100.27(3)^\circ$	Block, blue
$\gamma = 99.53(3)^\circ$	$0.32 \times 0.22 \times 0.18 \text{ mm}$
$V = 593.9(2) \text{ \AA}^3$	

### Data collection

Bruker CCD area-detector diffractometer	1971 independent reflections
$\omega$ scans	1470 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.040$
$T_{\text{min}} = 0.744$ , $T_{\text{max}} = 0.843$	$\theta_{\text{max}} = 25.0^\circ$
3094 measured reflections	$h = -8 \rightarrow 8$
	$k = -7 \rightarrow 8$
	$l = -14 \rightarrow 12$

### Refinement

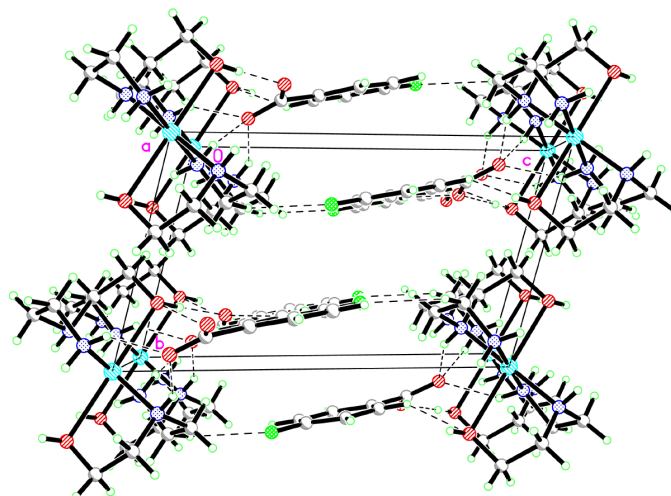
Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0946P)^2]$
$wR(F^2) = 0.168$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\text{max}} = 0.002$
1971 reflections	$\Delta\rho_{\text{max}} = 0.88 \text{ e \AA}^{-3}$
163 parameters	$\Delta\rho_{\text{min}} = -0.59 \text{ e \AA}^{-3}$

**Table 1**

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

Cu1—N2	2.004 (4)	Cu1—O1	2.443 (4)
Cu1—N1	2.044 (4)		
$N2^i$ —Cu1—N2	180	$N1$ —Cu1—O1 <sup>i</sup>	101.78 (15)
$N2$ —Cu1—N1 <sup>i</sup>	94.78 (17)	$N2$ —Cu1—O1	89.68 (15)
$N2$ —Cu1—N1	85.22 (17)	$N1$ —Cu1—O1	78.22 (15)
$N1^i$ —Cu1—N1	180	O1 <sup>i</sup> —Cu1—O1	180.00 (16)
$N2$ —Cu1—O1 <sup>i</sup>	90.32 (15)		

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



**Figure 2**

The crystal packing of (I), viewed along the  $a$  axis. Hydrogen bonds are indicated by dashed lines.

**Table 2**

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B $\cdots$ O3 <sup>iii</sup>	0.81 (8)	1.81 (8)	2.606 (6)	170 (9)
N2—H2B $\cdots$ O2 <sup>iii</sup>	0.90	2.16	3.025 (5)	161
N2—H2A $\cdots$ O2 <sup>iv</sup>	0.90	2.20	3.008 (6)	149
N1—H1A $\cdots$ O2 <sup>v</sup>	0.90	2.22	3.013 (6)	147

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

Atom H1B, attached to O1, was located in a difference map and its positional parameters were refined. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H distances of 0.90  $\text{\AA}$  and C—H distances in the range 0.96–0.97  $\text{\AA}$ . The  $U_{\text{iso}}$  values for atoms H11A, H11B, H2A and H2B were set equal to  $1.2U_{\text{eq}}(\text{C}, \text{N})$  and for the remaining H atoms the values were fixed at 0.08  $\text{\AA}^2$ . As a result of the large fraction of weak data at higher angles, the  $2\theta$  maximum was limited to  $50^\circ$ .

Data collection: SMART (Siemens, 1996); cell refinement: SAINT; data reduction: SAINT (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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