

**Krystyna Koćwin-Gieźak and  
Bernard Marciniak\***Institute of Chemistry and Environment  
Protection, Jan Długosz University, al. Armii  
Krajowej 13/15, 42-200 Częstochowa, Poland

Correspondence e-mail: k.gielzak@ajd.czest.pl

**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.046  
 $wR$  factor = 0.131  
Data-to-parameter ratio = 12.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**[4-(2-Aminoethyl)morpholine- $\kappa^2\text{N},\text{N}'$ ]aqua-  
(oxalato- $\kappa^2\text{O},\text{O}'$ )copper(II) monohydrate**

The crystal structure of the title compound,  $[\text{Cu}(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_{14}\text{N}_2\text{O})(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$ , includes a  $\text{CuN}_2\text{O}_3$  coordination polyhedron in the shape of a slightly distorted square pyramid with bidentate morpholine and oxalate ligands. Copper(II) is coordinated by 4-(2-aminoethyl)morpholine (etMorph) N atoms, with  $\text{Cu}-\text{N}$  distances of 2.050 (3) and 1.985 (3) Å, and two carboxylate O atoms from the oxalate ligand, with  $\text{Cu}-\text{O}$  distances of 1.955 (2) and 1.965 (2) Å; both ligands are located in the basal plane, whereas a water molecule is apically positioned [ $\text{Cu}-\text{O} = 2.251$  (3) Å]. The crystal packing is dominated by  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds.

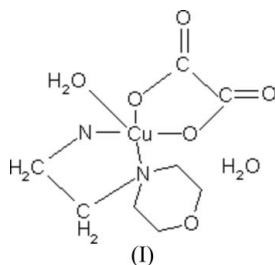
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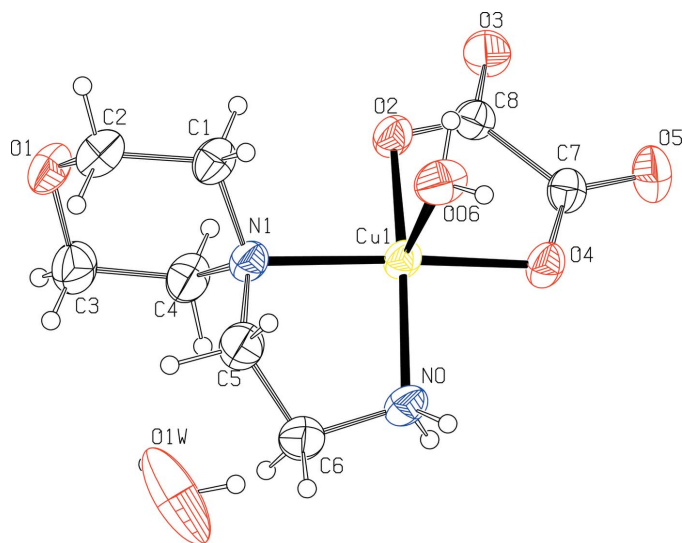
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**Comment**

Copper ions, present in naturally occurring systems, are involved in biochemical reactions. Morpholine can be used as a ligand in metal complexes but it can be a component of protective coatings on fresh fruits (McGuire & Hagenmaire, 1996) and used as an emulsifier in the preparation of pharmaceuticals and cosmetic products (Kuchowicz & Rydzynski, 1998). Its wide application is due to its relative safety for human health. Our initial aim was to investigate the activity of the  $[\text{Cu}(\text{L})_2]^{2+}$  complex where  $\text{L}$  is etMorph, *i.e.* 4-(2-aminoethyl)morpholine. In the synthesis we used different copper(II) salts, such as copper(II) chloride, nitrate and acetate with the same ligand; the products were all compound (I) (Fig. 1).



The  $\text{Cu}^{\text{II}}$  atom is slightly distorted square pyramidal with two N atoms from the etMorph ligand and two O atoms from the oxalate anion forming the basal plane, and atom O06 of the water molecule occupying the apical position (Fig. 2). The  $\text{Cu}-\text{O}06$  apical bond (2.252 Å) is shorter than the reported values for complexes with heterocyclic amines and malonate as ligands, and significantly shorter than in other oxalate complexes (Bouayad *et al.*, 1995). The coordination geometry around the  $\text{Cu}^{\text{II}}$  atom is similar to those in some reported  $\text{CuN}_2\text{O}_3$ -type complexes, for example  $[\text{Cu}(\text{bpym})(\text{mal})(\text{H}_2\text{O})]\cdot 6\text{H}_2\text{O}$  (Rodríguez-Martin *et al.*, 2001),  $[\text{Cu}(\text{mal})(-$



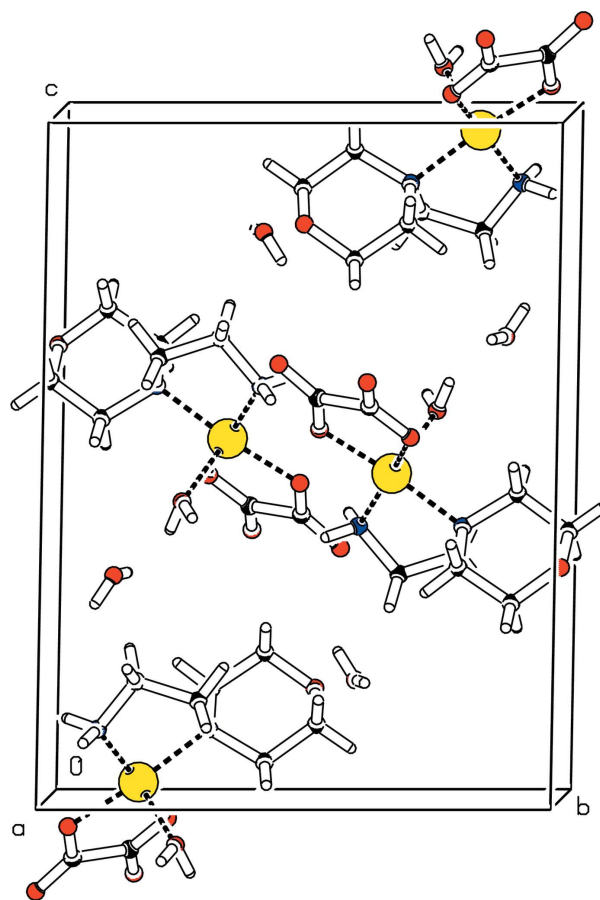
**Figure 1**  
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

phen)(H<sub>2</sub>O)] (Kwik *et al.*, 1986), [Cu(mal)-(bpy)(H<sub>2</sub>O)] (Lu *et al.*, 1996), [Cu(mal)(bpy)(H<sub>2</sub>O)]·H<sub>2</sub>O (Suresh *et al.*, 1997), [Cu(mal)(dmp)<sub>2</sub>(H<sub>2</sub>O)] (Xiong *et al.*, 2001) (phen is 1,10-phenanthroline, bpy is 2,2'-bipyridine, bpm is 2,2'-bipyrimidine, dmp is 3,5-dimethyl-1*H*-pyrazole and mal is malonic acid).

In the crystal structure, molecules are linked by: (i) N—H···O hydrogen bonds in which the morpholine ligand is a double donor to oxalate O atoms (coordinated and uncoordinated); (ii) O—H···O hydrogen bonds in which an uncoordinated water molecule, O1W, acts as donor to oxalate O atom O5 and morpholine O atom O1; (iii) the coordinated water O06 which is a donor to the uncoordinated water and uncoordinated oxalate O atom O3 (Table 2). Graph-set analysis (Bernstein *et al.*, 1995) performed by the computer program *RPLUTO* (Motherwell *et al.*, 2000) indicated that the uncoordinated and coordinated water molecules O1W···O5 (a in Fig. 3), O1W···O1 (b in Fig. 3) and O06···O1W (c in Fig. 3) form discrete *D* motifs. O06—H···O3 (d in Fig. 3) links the complex molecules by translation along the *a* axis into a *C*(6) chain. N0···O4 (e in Fig. 3) and N0···O3 (f in Fig. 3) form rings with graph-set motifs *R*<sub>2</sub><sup>2</sup>(8) and *R*<sub>2</sub><sup>2</sup>(12), respectively. Apart from these hydrogen bonds, in the structure of (I) there is also a weak intermolecular hydrogen bond of type C—H···O (g in Fig. 3) which connects the morpholine ring with the oxalate anion into a ring defined by the *R*<sub>2</sub><sup>2</sup>(14) descriptor.

## Experimental

To a warm aqueous solution of copper(II) acetate (0.05 mol, 0.998 g) dissolved in 30 ml of water, etMorph (0.34 ml, 0.1 mol) and then an ammonium oxalate (0.713 g, 0.05 mol) solution in 10 ml of water were added slowly with stirring. The mixture was warmed to 333 K and stirred for 30 min. Blue crystals of the title compound appeared within 3 d. Identical crystals were obtained using copper(II) chloride or nitrate instead of copper(II) acetate.



**Figure 2**  
The crystal packing, viewed approximately along the *a* axis.

### Crystal data

[Cu(C<sub>2</sub>O<sub>4</sub>)(C<sub>6</sub>H<sub>14</sub>N<sub>2</sub>O)(H<sub>2</sub>O)]·H<sub>2</sub>O  
*M<sub>r</sub>* = 317.79  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 6.8240 (14) Å  
*b* = 11.916 (2) Å  
*c* = 16.396 (3) Å  
 $\beta$  = 108.76 (3)°  
*V* = 1262.4 (5) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.672 Mg m<sup>-3</sup>  
 Cu *K*α radiation  
 Cell parameters from 30 reflections  
 $\theta$  = 6–25°  
 $\mu$  = 2.75 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Column, blue  
 0.35 × 0.10 × 0.06 mm

### Data collection

Kuma KM-4 diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction: part of the refinement model ( $\Delta F$ ) (*DIFABS*; Walker & Stuart, 1983)  
*T*<sub>min</sub> = 0.755, *T*<sub>max</sub> = 0.838  
 2315 measured reflections  
 2315 independent reflections

1968 reflections with *I* > 2σ(*I*)  
 $\theta$ <sub>max</sub> = 68.5°  
*h* = -8 → 8  
*k* = -14 → 0  
*l* = -19 → 7  
 3 standard reflections  
 frequency: 100 min  
 intensity decay: 1.2%

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.046  
*wR*(*F*<sup>2</sup>) = 0.131  
*S* = 1.06  
 2315 reflections  
 187 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.8891P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.034$   
 $\Delta\rho_{\max} = 0.41 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{Å}^{-3}$

**Table 1**  
Selected geometric parameters (Å, °).

Cu1—O2	1.955 (2)	N1—C5	1.485 (5)
Cu1—O4	1.965 (2)	N1—C1	1.492 (4)
Cu1—N0	1.985 (3)	N1—C4	1.493 (5)
Cu1—N1	2.050 (3)	O3—C8	1.230 (4)
Cu1—O06	2.252 (3)	O4—C7	1.268 (4)
O2—C8	1.263 (4)	C7—O5	1.225 (4)
O2—Cu1—O4	84.18 (10)	N0—Cu1—N1	86.52 (12)
O2—Cu1—N0	161.99 (13)	O2—Cu1—O06	98.55 (11)
O4—Cu1—N0	92.53 (12)	O4—Cu1—O06	95.90 (11)
O2—Cu1—N1	94.75 (11)	N0—Cu1—O06	99.40 (13)
O4—Cu1—N1	173.50 (11)	N1—Cu1—O06	90.60 (12)

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1W—H1WA···O5 <sup>i</sup>	0.80 (2)	1.96 (3)	2.706 (5)	154 (5)
N0—H0A···O4 <sup>ii</sup>	0.88 (4)	2.15 (2)	3.002 (4)	163 (4)
N0—H0B···O3 <sup>i</sup>	0.86 (2)	2.37 (2)	3.218 (4)	170 (4)
O1W—H1WB···O1 <sup>iii</sup>	0.82 (7)	2.25 (9)	2.729 (5)	118 (8)
O06—H06A···O1W <sup>iv</sup>	0.82 (2)	1.91 (3)	2.679 (5)	156 (5)
O06—H06B···O3 <sup>v</sup>	0.82 (5)	1.90 (5)	2.702 (4)	169 (6)
C4—H4B···O5 <sup>i</sup>	0.97	2.57	3.227 (5)	126

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

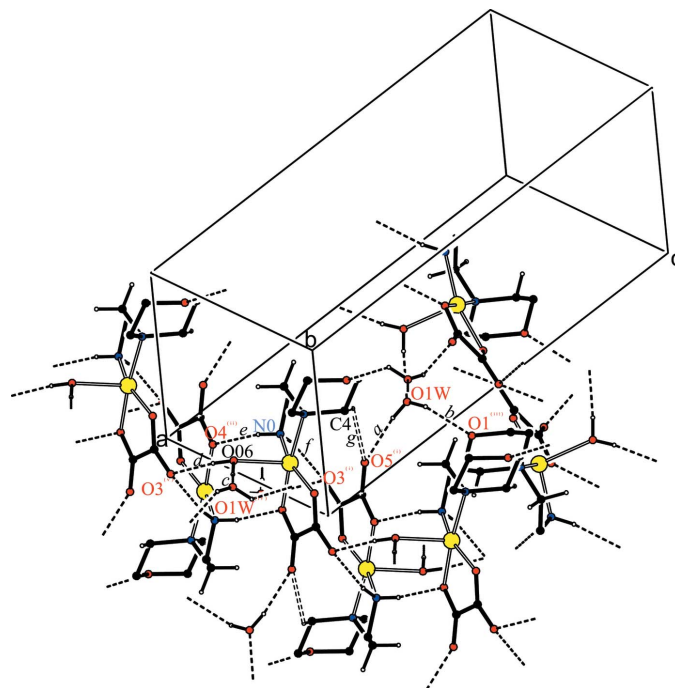
All H atoms bound to C atoms were treated as riding, with C—H = 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H atoms bound to O and N atoms were located in a difference Fourier map and refined with O—H and N—H distance restraints of 0.82 (2) and 0.87 (2) Å, respectively.

Data collection: *KM4B8 Software* (Galdecki *et al.*, 1996); cell refinement: *KM4B8 Software*; data reduction: *KM4B8 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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**Figure 3**  
The hydrogen-bond network in the structure of (I), showing O—H···O (*a–d*), N—H···O (*e* and *f*) and C—H···O (*g*, double dashed lines) interactions. H atoms not involved in these interactions have been omitted for clarity.

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