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#### Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
R factor = 0.044  
wR factor = 0.116  
Data-to-parameter ratio = 14.1

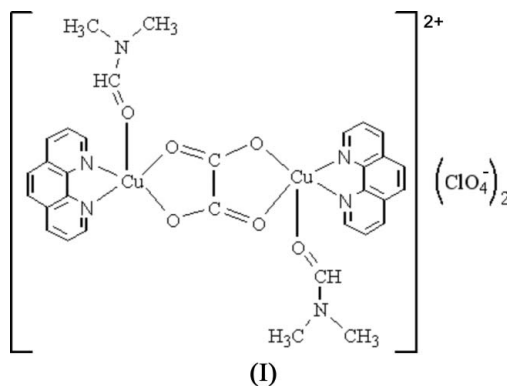
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## $\mu$ -Oxalato-bis[(N,N'-dimethylformamide)(1,10-phenanthroline)copper(II)] bis(perchlorate)

The title centrosymmetric binuclear complex,  $[\text{Cu}_2(\text{C}_2\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_3\text{H}_7\text{NO})_2](\text{ClO}_4)_2$ , was synthesized by the reaction of 1,10-phenanthroline, 2,5-dihydroxy-1,4-dithiane and  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ . In the asymmetric unit, the  $\text{Cu}^{\text{II}}$  atom is in a distorted square-pyramidal coordination geometry. The closest  $\text{Cu} \cdots \text{O}$  distance involving the perchlorate anion is  $2.745(2) \text{ \AA}$ .

#### Comment

Binuclear copper(II) complexes with 1,10-phenanthroline and carboxylate bridging ligands have been found to be important in some metalloenzymes such as urease. These units can cleave DNA under physiological conditions and catalyze the hydrolysis of urease to form ammonia and carbamate (Person *et al.*, 1997; Jabri *et al.*, 1995; Thomas *et al.*, 2002). Recently, several binuclear complexes have been prepared as models for urease in order to explore the area of hydrolysis (Sung *et al.*, 2001; Barrios & Lippard, 1999; Barrios & Lippard, 2000). However, only a few copper binuclear carboxylate complexes have been structurally characterized. In the present study, we used the potentially bridging oxalate ligand to prepare the title binuclear complex, (I).



In the asymmetric unit of (I), a  $\text{Cu}^{\text{II}}$  atom is coordinated in a distorted square-pyramidal geometry defined by two N atoms from a 1,10-phenanthroline ligand and two O atoms from an oxalate ligand in the basal plane, and by an O atom from a dimethylformamide ligand in the apical position. The complete molecular structure is generated by crystallographic inversion symmetry (Fig. 1). The value (Albada *et al.*, 1999) of  $\tau = (173.88 - 171.53)/60 = 0.0392$  indicates the degree of distortion from ideal square-pyramidal geometry. The distance between two  $\text{Cu}^{\text{II}}$  atoms within a cation is  $5.134(2) \text{ \AA}$ . Selected bond lengths and angles are given in Table 1. The  $\text{Cu}-\text{O}$  and  $\text{Cu} \cdots \text{Cu}$  distances in (I) agree with those in

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$[[\text{CuL}(\text{H}_2\text{O})_2(\mu^4\text{-oxa})](\text{ClO}_4)_2$ , (II), (Thomas *et al.*, 2002). As in (II), there is a longer Cu...O contact [2.745 (2) Å in (I) for Cu1...O4] between a Cu<sup>II</sup> atom and an O atom from a perchlorate anion, which likely involves a weak bonding interaction.

**Experimental**

A mixture of  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  (0.1114 g, 0.30 mmol), 1,10-phenanthroline (0.0598 g, 0.45 mmol) and 2,5-dihydroxy-1,4-dithiane (0.0454 g, 0.30 mmol) was dissolved in *N,N'*-dimethylformamide (10 ml) and methanol (10 ml). Blue prismatic crystals of (I) separated from the solution after 10 d.

*Crystal data*

$[\text{Cu}_2(\text{C}_2\text{O}_4)(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_3\text{H}_7\text{NFO})_2](\text{ClO}_4)_2$   
 $M_r = 920.62$   
 Triclinic,  $P\bar{1}$   
 $a = 8.3567$  (11) Å  
 $b = 9.2013$  (12) Å  
 $c = 11.7229$  (15) Å  
 $\alpha = 84.321$  (17)°  
 $\beta = 86.979$  (17)°  
 $\gamma = 81.809$  (17)°  
 $V = 887.1$  (2) Å<sup>3</sup>  
 $Z = 1$   
 $D_x = 1.723$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 1.43$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, blue  
 0.12 × 0.10 × 0.06 mm

*Data collection*

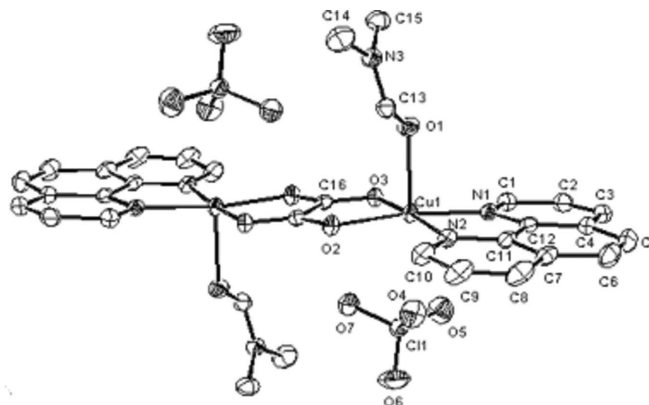
Bruker SMART APEX CCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.847$ ,  $T_{\max} = 0.919$   
 7265 measured reflections  
 3634 independent reflections  
 2941 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\text{max}} = 26.5^\circ$

*Refinement*

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.116$   
 $S = 1.03$   
 3634 reflections  
 257 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.0846P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

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

Cu1—O3	1.966 (2)	Cu1—N1	1.991 (3)
Cu1—O2	1.970 (2)	Cu1—O1	2.289 (2)
Cu1—N2	1.988 (3)		
O3—Cu1—O2	85.20 (9)	N2—Cu1—N1	83.08 (11)
O3—Cu1—N2	173.88 (10)	O3—Cu1—O1	89.32 (9)
O2—Cu1—N2	94.33 (10)	O2—Cu1—O1	93.71 (9)
O3—Cu1—N1	96.51 (10)	N2—Cu1—O1	96.79 (10)
O2—Cu1—N1	171.53 (10)	N1—Cu1—O1	94.61 (9)



**Figure 1**

Structure of (I), showing displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted and unlabeled atoms are related to labeled atoms by the symmetry operator  $(-x, 1 - y, 1 - z)$ .

Atom H13 was refined independently with an isotropic displacement parameter [ $\text{C13—H13} = 0.96$  (4) Å]. All other H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with  $\text{C—H} = 0.93$  or  $0.96$  Å (for methyl H atoms) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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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