

Di- $\mu$ -methoxy-bis[dipyridinecopper(II)] diperchlorate

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## Key indicators

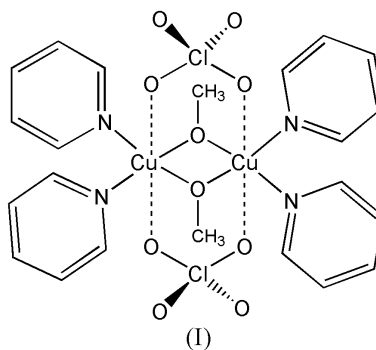
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.033  
 $wR$  factor = 0.095  
Data-to-parameter ratio = 14.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound,  $[\text{Cu}_2(\text{CH}_3\text{O})_2(\text{C}_5\text{H}_5\text{N})_4](\text{ClO}_4)_2$ , consists of a centrosymmetric dinuclear unit with bridging methoxy groups, and each  $\text{Cu}^{\text{II}}$  atom forms a square-planar  $\text{CuN}_2\text{O}_2$  unit with pyridine ligands. The  $\text{Cu}\cdots\text{Cu}$  distance is 2.9336 (11) Å and the  $\text{Cu}-\text{O}-\text{Cu}$  bond angle is 99.51 (7)°. The perchlorate anions are at semi-coordination distances, the  $\text{Cu}-\text{O}(\text{perchlorate})$  distances being in the range 2.649 (2)–2.741 (2) Å.

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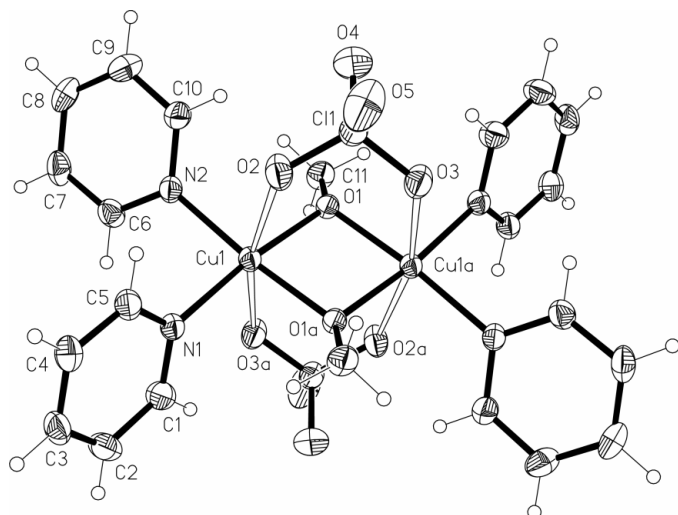
## Comment

There has been much interest in recent years in planar  $\text{Cu}(\mu\text{-OR})-\text{Cu}$  dinuclear systems because of the magnetostructural correlation between the  $\text{Cu}-\text{O}-\text{Cu}$  bond angle and the magnetic exchange parameter (Graham *et al.*, 2001; Hatfield, 1984; Ruiz *et al.*, 1997). The title complex, (I), was obtained in an attempt to prepare a polymeric copper complex of 5,5'-thiodisalicylate.



The title compound, (I), is a centrosymmetric dinuclear  $\text{Cu}^{\text{II}}$  complex (Fig. 1). Each Cu atom shows square-planar coordination, with the basal plane formed by the two pyridine N atoms and two methoxy O atoms. The  $\text{Cu}-\text{O}$  and  $\text{Cu}-\text{N}$  distances are 1.9170 (18)–1.9263 (18) Å and 1.992 (2)–2.002 (2) Å, respectively; these values are comparable to those in similar compounds. However, the  $\text{Cu}\cdots\text{Cu}$  distance and  $\text{Cu}-\text{O}-\text{Cu}$  bond angle significantly exceed the range for similar compounds reported in the literature. The  $\text{Cu}1\cdots\text{Cu}1^i$  distance [symmetry code: (i)  $-2-x, 1-y, -2-z$ ] of 2.9336 (11) Å and the  $\text{Cu}1-\text{O}1-\text{Cu}1^i$  bond angle of 99.51 (7)° are shorter and smaller than those in comparable dinuclear square-planar copper(II) compounds [2.974 (1)–3.034 (1) Å and 101.72 (7)–103.97 (9)°; Bu *et al.*, 2004; Komaei *et al.*, 1999; Wang *et al.*, 2001].

The perchlorate anion in (I) is bridging, at semi-coordination distances [2.649 (2) and 2.741 (2) Å] that are similar to



**Figure 1**  
Molecular structure of (I), showing 50% probability displacement ellipsoids. Atoms labelled with the suffix a are at the symmetry position  $(-2-x, 1-y, -2-z)$ .

those in bis( $\mu$ -methoxy)tetrakis(2-amino-5-picolinyl)diperoxocuprate(II) (Komaei *et al.*, 1999).

## Experimental

Copper(II) nitrate (0.242 g, 1.0 mmol) and 5,5'-thiodisalicyclic acid (0.153 g, 0.5 mmol) were placed in a 10:1 (*v/v*) methanol/pyridine mixture and the solution was heated until the reagents dissolved. A solution (2 ml) of  $\text{NaClO}_4$  (0.142 g, 1.0 mmol) was then added. Purple block-shaped crystals of (I) separated from the solution in about 20% yield after 3 d.

### Crystal data

$[\text{Cu}_2(\text{CH}_3\text{O})_2(\text{C}_5\text{H}_5\text{N})_4](\text{ClO}_4)_2$   
 $M_r = 704.45$   
 Monoclinic,  $P2_1/n$   
 $a = 8.528$  (4) Å  
 $b = 16.850$  (9) Å  
 $c = 10.185$  (6) Å  
 $\beta = 108.697$  (8)°  
 $V = 1386.3$  (13) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.688$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 4713 reflections  
 $\theta = 3.2$ – $27.5$ °  
 $\mu = 1.79$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, purple  
 $0.38 \times 0.32 \times 0.24$  mm

### Data collection

Rigaku Mercury CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2002)  
 $T_{\min} = 0.512$ ,  $T_{\max} = 0.651$   
 8628 measured reflections

2666 independent reflections  
 2230 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$   
 $\theta_{\text{max}} = 26.0$ °  
 $h = -9 \rightarrow 10$   
 $k = -20 \rightarrow 20$   
 $l = -12 \rightarrow 10$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.096$   
 $S = 1.09$   
 2666 reflections  
 181 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0576P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.49$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O1	1.9170 (18)	Cu1—O2	2.649 (2)
Cu1—O1 <sup>i</sup>	1.9263 (18)	Cu1—O3 <sup>i</sup>	2.741 (2)
Cu1—N1	1.992 (2)	Cu1—Cu1 <sup>i</sup>	2.9336 (11)
Cu1—N2	2.002 (2)		
O1—Cu1—O1 <sup>i</sup>	80.49 (7)	O1 <sup>i</sup> —Cu1—N2	174.91 (7)
O1—Cu1—N1	173.69 (7)	N1—Cu1—N2	91.08 (9)
O1 <sup>i</sup> —Cu1—N1	93.60 (8)	Cu1—O1—Cu1 <sup>i</sup>	99.51 (7)

Symmetry code: (i)  $-2-x, 1-y, -2-z$ .

All H atoms were included in calculated positions and constrained to ride at a distance of 0.93 Å from their parent C atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , for the pyridyl groups and 0.96 Å from their parent C atoms, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ , for the methyl group.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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