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Di-μ-methoxo-bis[dipyridinecopper(II)] diperchlorate

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The title compound, $[Cu_2(CH_3O)_2(C_5H_5N)_4](ClO_4)_2$, consists of a centrosymmetric dinuclear unit with bridging methoxo groups, and each Cu^{II} atom forms a square-planar CuN_2O_2 unit with pyridine ligands. The Cu$\cdots$Cu distance is 2.9336 (11) Å and the Cu—O—Cu bond angle is 99.51 (7)°. The perchlorate anions are at semi-coordination distances, the Cu—O(perchlorate) distances being in the range 2.649 (2)–2.741 (2) Å.

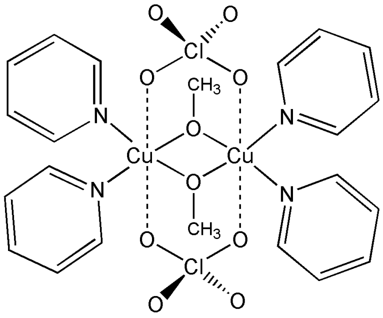
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.095
Data-to-parameter ratio = 14.7

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

Comment

There has been much interest in recent years in planar Cu—(μ-OR)—Cu dinuclear systems because of the magnetostructural correlation between the Cu—O—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.



(I)

The title compound, (I), is a centrosymmetric dinuclear Cu^{II} complex (Fig. 1). Each Cu atom shows square-planar coordination, with the basal plane formed by the two pyridine N atoms and two methoxo O atoms. The Cu—O and Cu—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 Cu$\cdots$Cu distance and Cu—O—Cu bond angle significantly exceed the range for similar compounds reported in the literature. The Cu1$\cdots$Cu1^{i} distance [symmetry code: (i) $-2-x$, $1-y$, $-2-z$] of 2.9336 (11) Å and the Cu1—O1—Cu1^{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

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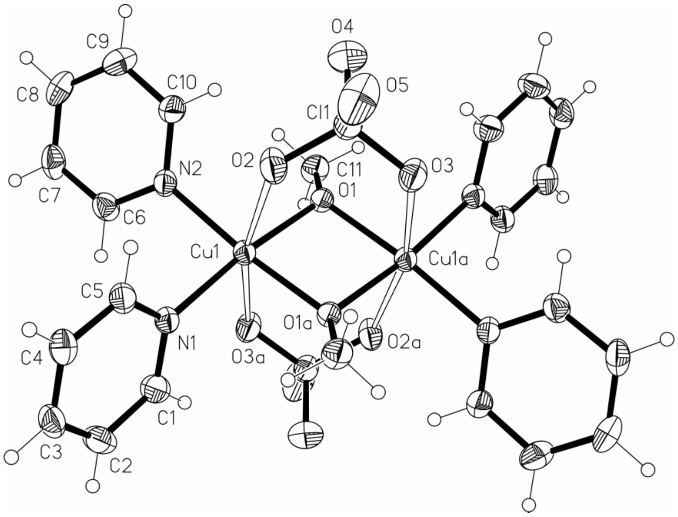

Figure 1
Molecular structure of (I), showing 50% probability displacement ellipsoids. Atoms labelled with the suffix a are at the symmetry position $(-2 - x, 1 - y, -2 - z)$.

those in bis(μ-methoxo)tetrakis(2-amino-5-picolinyl)dicopper(II) diperchlorate (Komaei *et al.*, 1999).

Experimental

Copper(II) nitrate (0.242 g, 1.0 mmol) and 5,5′-thiodisalicylic 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 $NaClO_4$ (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

$[Cu_2(CH_3O)_2(C_5H_5N)_4](ClO_4)_2$
$M_r = 704.45$
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^3
$Z = 2$

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

Data collection

Rigaku Mercury CCD diffractometer
ω 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 $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.0°$
$h = -9 \rightarrow 10$
$k = -20 \rightarrow 20$
$l = -12 \rightarrow 10$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9170 (18)	Cu1—O2	2.649 (2)
Cu1—O1^i	1.9263 (18)	Cu1—O3^i	2.741 (2)
Cu1—N1	1.992 (2)	Cu1—Cu1^i	2.9336 (11)
Cu1—N2	2.002 (2)		
O1—Cu1—O1^i	80.49 (7)	O1^i—Cu1—N2	174.91 (7)
O1—Cu1—N1	173.69 (7)	N1—Cu1—N2	91.08 (9)
O1^i—Cu1—N1	93.60 (8)	Cu1—O1—Cu1^i	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 $U_{iso}(H) = 1.2U_{eq}(C)$, for the pyridyl groups and 0.96 Å from their parent C atoms, with $U_{iso}(H) = 1.5U_{eq}(C)$, for the methyl group.

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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