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Bis(μ-4-methoxypyridine *N*-oxide-κ^2O:*O*)-bis[dibromocopper(II)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.014 Å
R factor = 0.068
wR factor = 0.153
Data-to-parameter ratio = 15.1

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

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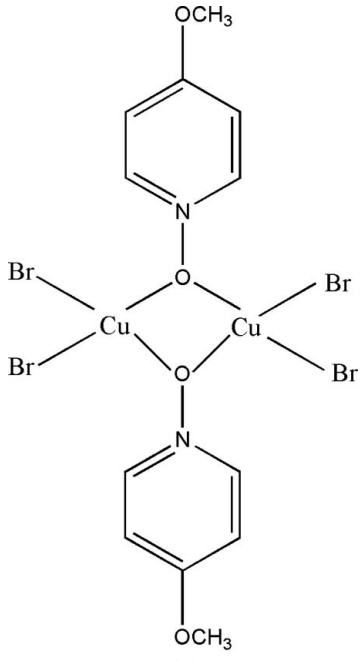
In the binuclear centrosymmetric title compound, $[Cu_2Br_4(C_6H_7NO_2)_2]$, two 4-methoxypyridine *N*-oxide ligands bridge two Cu atoms, conferring a square-planar geometry on Cu. Hydrogen bonds of the C—H···Br type lead to the formation of a sheet structure.

Comment

Aromatic *N*-oxides are useful bridging ligands and a large number of multinuclear complexes have these ligands exhibiting this feature. Some have magnetic coupling properties (Watson, 1969). As we have previously synthesized complexes with pyridine *N*-oxide and its derivatives (Shi *et al.*, 2006), our studies continue with the title centrosymmetric binuclear copper complex, (I) (Fig. 1).



(I)

The Cu atom of (I) assumes a square-planar geometry. The two 4-methoxypyridine *N*-oxide ligands function as bridging ligands. The Cu···Cu distance is 3.251 (2) Å. Atom Cu1 lies within the square plane and the maximum deviation is 0.104 (5) Å for atom Br2. The compound may show magnetic interaction (magnetic exchange or magnetic coupling), as noted from the angle at the bridging O atom (Nepveu *et al.*, 1986).

Non-classical hydrogen bonds (Table 2) lead to the formation of a sheet parallel to the *bc* plane.

Experimental

4-Methoxypyridine *N*-oxide (0.1165 g, 0.931 mmol) in water (15 ml) was added to an aqueous solution (10 ml) of $Cu(ClO_4)_2{\cdot}6H_2O$ (0.3461 g, 0.934 mmol) and NaBr (0.1918 g, 1.86 mmol). The solution was stirred for a few minutes. Red single crystals of (I) were obtained after a month.

Crystal data

$[Cu_2Br_4(C_6H_7NO_2)_2]$
M_r = 696.97
Monoclinic, $P2_1/c$
a = 12.102 (3) Å
b = 10.054 (3) Å
c = 7.767 (2) Å
β = 90.962 (4)°
V = 944.9 (4) Å^3
Z = 2
D_x = 2.450 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 10.73 mm^{-1}
T = 298 (2) K
Prism, red
0.15 × 0.12 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.296, T_{max} = 0.565
(expected range = 0.275–0.525)
4667 measured reflections
1664 independent reflections
1391 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.153
S = 1.13
1664 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.989 (6)	Cu1—Br2	2.3411 (16)
Cu1—Br1	2.3368 (15)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H1···Br1^{i}	0.93	2.92	3.744 (9)	148
C6—H6B···Br2^{ii}	0.96	2.90	3.790 (12)	156

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x-1, -y+\frac{3}{2}, z+\frac{1}{2}$.

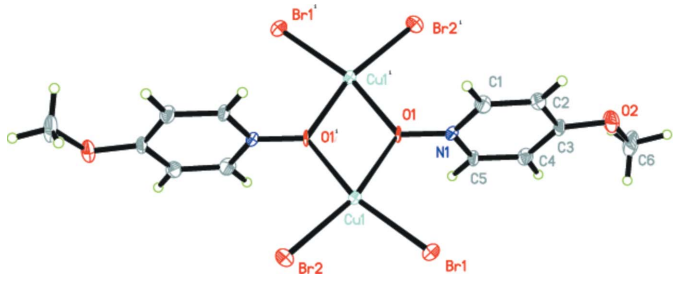


Figure 1
The molecular structure of (I), showing the atom-numbering scheme, with Displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $-x+1, -y+1, -z$.]

The H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for the pyridine ring, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group. The highest peak is located 0.91 Å from atom Br2.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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