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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.012$ Å
Disorder in main residue
 R factor = 0.059
 wR factor = 0.160
Data-to-parameter ratio = 14.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dibromobis(3-methoxy-2-methylpyrazine 1-oxide- κO)copper(II)

In the title mononuclear Cu^{II} complex, $[\text{CuBr}_2(\text{C}_6\text{H}_8\text{N}_2\text{O}_2)_2]$, the Cu^{II} atom assumes a tetrahedrally distorted square-planar coordination geometry. Two Br^- anions and two methylmethoxy pyrazine oxide ligands (mmpo) coordinate in a *cis* manner to the Cu^{II} atom, with a dihedral angle of 34.60 (16) $^\circ$ the between the $\text{Cu}/\text{Br}/\text{Br}$ and $\text{Cu}/\text{O}/\text{O}$ planes.

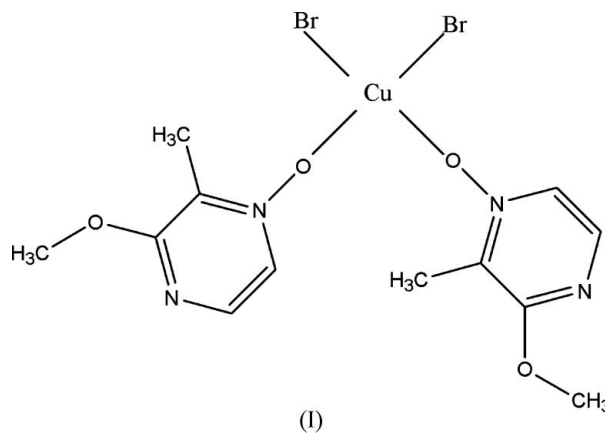
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Comment

Pyrazine *N*-oxide and its derivatives usually play the role of bridge ligands in polynuclear metal complexes (Sun *et al.*, 2001). We prepared the title Cu^{II} complex, (I), incorporating a methylmethoxy pyrazine oxide ligand. Its X-ray crystal structure shows a monodentate coordination mode for the pyrazine *N* oxide ligand.



The molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom assumes a tetrahedrally distorted square-planar coordination geometry. Two methylmethoxy pyrazine oxide (mmpo) ligands coordinate *cis* to the Cu^{II} atom *via* the terminal O atom, but not *via* the pyrazine N atoms. Thus, mmpo displays a monodentate coordination mode in (I). Two Br^- anions are bonded to the Cu^{II} atom to complete the four-coordinate geometry. The $\text{Cu}/\text{O}1/\text{O}3$ plane is tilted with respect to the $\text{Cu}/\text{Br}1/\text{Br}2$ plane by a dihedral angle of 34.60 (16) $^\circ$. The bond angles at the Cu atom (Table 1) also show the extent of the distortion of the coordination geometry from square planar.

Of the two coordinated mmpo ligands, one is ordered but the other one is disordered over two different orientations, as shown in Fig. 1.

Experimental

3-Methoxy-2-methylpyrazine 1-oxide (0.23 g, 1.7 mmol) was added to an aqueous solution (15 ml) containing $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.31 g,

0.85 mmol) and NaBr (0.18 g, 1.7 mmol). The solution was stirred for 10 min at room temperature. Red single crystals of (I) were obtained after three weeks.

Crystal data

[CuBr₂(C₆H₈N₂O₂)₂]

M_r = 503.65

Triclinic, *P*1

a = 8.270 (2) Å

b = 10.619 (3) Å

c = 11.399 (3) Å

α = 64.657 (3)°

β = 75.794 (4)°

γ = 72.154 (4)°

V = 853.6 (4) Å³

Z = 2

D_x = 1.960 Mg m⁻³

Mo *K*α radiation

Cell parameters from 1930

reflections

θ = 2.3–26.7°

μ = 5.98 mm⁻¹

T = 298 (2) K

Prism, red

0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

T_{min} = 0.437, *T_{max}* = 0.556

4443 measured reflections

2956 independent reflections

2343 reflections with *I* > 2σ(*I*)

R_{int} = 0.025

θ_{max} = 25.0°

h = -5 → 9

k = -12 → 12

l = -13 → 13

Refinement

Refinement on *F*²

R [*F*² > 2σ(*F*²)] = 0.059

wR (*F*²) = 0.160

S = 1.07

2956 reflections

202 parameters

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0867*P*)²

+ 2.2242*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/*σ*)_{max} < 0.001

Δρ_{max} = 1.48 e Å⁻³

Δρ_{min} = -0.76 e Å⁻³

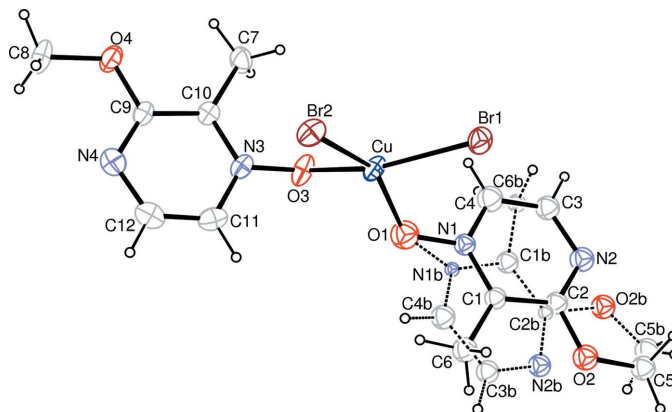


Figure 1

The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The dashed lines indicate the minor component of the disordered mmpo ligand.

refinement. Both components of the disordered mmpo ligand were refined isotropically. Methyl H atoms were placed in calculated positions (C–H = 0.96 Å) and refined with *U*_{iso}(H) = 1.5*U*_{eq}(C). Other H atoms were placed in calculated positions with C–H = 0.93 Å and refined using a riding model, with *U*_{iso}(H) = 1.2*U*_{eq}(C). The highest peak in the difference map is 0.90 Å from atom Br2.

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: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|-------------|-----------|-------------|
| Cu–Br1 | 2.3584 (13) | Cu–O1 | 1.970 (6) |
| Cu–Br2 | 2.3651 (12) | Cu–O3 | 1.959 (5) |
| Br1–Cu–Br2 | 97.33 (4) | Br2–Cu–O1 | 151.85 (18) |
| Br1–Cu–O1 | 95.44 (19) | Br2–Cu–O3 | 96.22 (14) |
| Br1–Cu–O3 | 157.67 (17) | O1–Cu–O3 | 80.5 (2) |

In the initial refinement process, the larger displacement parameters and some residual electron-density peaks implied a disordered structure for one mmpo ligand. The minor component of the mmpo ligand was located in a difference Fourier map. Occupancies were refined using the SUMP command and converged to 0.782 (3) and 0.218 (3). They were then fixed as 0.78 and 0.22 in the final cycles of

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