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Dibromobis(4-methoxypyridine *N*-oxide-κO)zinc(II)

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Key indicators

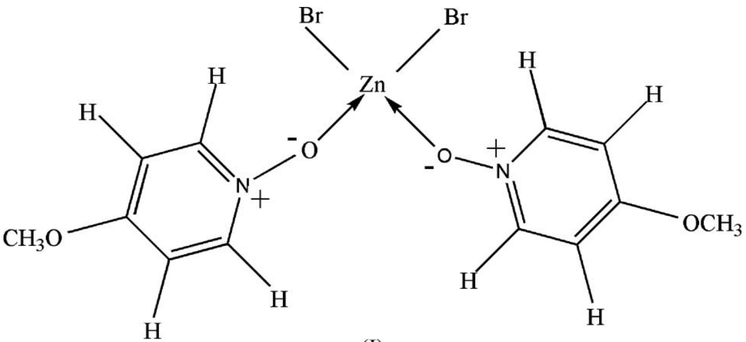
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 14.8

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

In the title mononuclear complex, $[ZnBr_2(C_6H_7NO_2)_2]$, the Zn^{II} atom is coordinated by two Br and two O atoms in a distorted tetrahedral geometry. There are π–π stacking interactions between the 4-methoxypridine *N*-oxide units.

Comment

Pyridine *N*-oxide and its derivatives usually act as bridging and terminal ligands, and a large number of complexes have been prepared with those ligands (Watson, 1969; Shi, 2005). We report here the synthesis and the structure of the title Zn^{II} complex, (I) (Fig. 1).



(I)

The Zn^{II} atom assumes a distorted $ZnBr_2O_2$ tetrahedral coordination geometry (Table 1), where the dihedral angle between the Zn/Br/Br and Zn/O/O planes is 88.18 (10)°. There are significant π–π stacking interactions between neighbouring pyridine rings; the relevant distances are $Cg1\cdots Cg1^{i}$ = 4.335 (3) Å and $Cg1\cdots 1^{i}_{perp}$ = 3.563 Å, and $Cg2\cdots Cg2^{ii}$ =

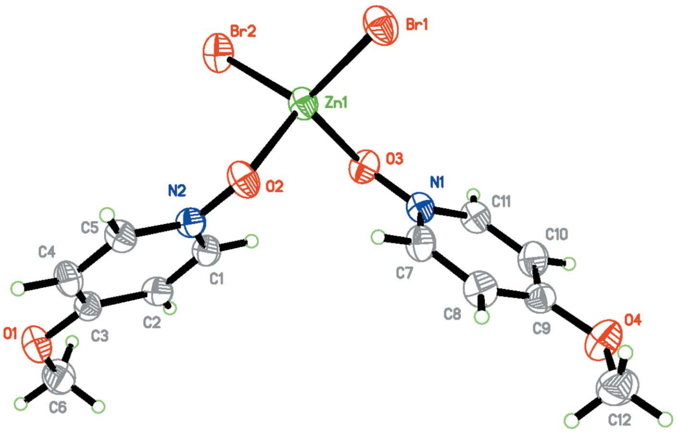


Figure 1
View of complex (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids.

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3.590 (3) Å and $Cg2\cdots2^{\rm ii}_{\rm perp}$ = 3.559 Å [symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $2 - x, 1 - y, -z$; *Cg*1 and *Cg*2 are the centroids of the N1/C7–C11 and N2/C1–C5 rings, respectively; $CgI\cdots J_{\rm perp}$ is the perpendicular distance from *CgI* to ring *J*].

Experimental

4-Methoxypyridine *N*-oxide (0.1025 g, 0.819 mmol, in 15 ml H_2O) was added to an aqueous solution (10 ml) containing $Zn(ClO_4)_2\cdot6H_2O$ (0.1573 g, 0.422 mmol) and NaBr (0.0873 g, 0.848 mmol). The resulting solution was stirred for a few minutes. Colourless single crystals were obtained after the solution had been allowed to stand at room temperature for three weeks.

Crystal data

$[ZnBr_2(C_6H_7NO_2)_2]$
M_r = 475.44
Triclinic, $P\overline{1}$
a = 7.1783 (18) Å
b = 8.501 (2) Å
c = 14.108 (3) Å
α = 78.294 (3)°
β = 76.293 (3)°
γ = 83.317 (4)°
V = 816.9 (3) Å^3
Z = 2
D_x = 1.933 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1347 reflections
θ = 2.5–23.8°
μ = 6.41 mm^{-1}
T = 298 (2) K
Prism, colourless
0.23 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.298, $T_{\rm max}$ = 0.527
4287 measured reflections
2846 independent reflections
2115 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021
$\theta_{\rm max}$ = 25.1°
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 6$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.102
S = 0.99
2846 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.62 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3	1.980 (3)	Zn1—Br1	2.3267 (9)
Zn1—O2	2.022 (3)	Zn1—Br2	2.3565 (10)
O3—Zn1—O2	104.29 (14)	O3—Zn1—Br2	104.88 (10)
O3—Zn1—Br1	110.95 (10)	O2—Zn1—Br2	106.35 (10)
O2—Zn1—Br1	106.89 (10)	Br1—Zn1—Br2	122.08 (3)

All H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for pyridine H atoms, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H atoms.

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* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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