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Diiodidobis(4-methylpyridine *N*-oxide-κO)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.030
wR factor = 0.075
Data-to-parameter ratio = 18.1

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

The title mononuclear complex, $[Zn(I)_2(C_6H_7NO)_2]$, lies on a special position of site symmetry 2. The Zn atom is coordinated by two I and two O atoms in a tetrahedral geometry. There is a π–π stacking interaction of the 4-methylpyridine *N*-oxide units.

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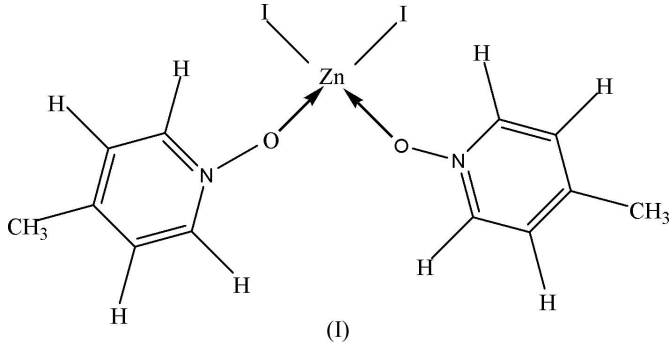
Comment

In the title molecular complex, (I), (Fig. 1), the Zn atom is coordinated by two I atoms and the O atoms from two 4-methylpyridine *N*-oxide ligands. Atom Zn1 lies on a twofold axis in a distorted tetrahedral environment. The 4-methylpyridine *N*-oxide units are stacked over each other at a distance of about 3.66 Å. Such π–π stacking causes the molecules to pack as columns along the *b* axis.



(I)

Experimental

4-Methylpyridin *N*-dioxide (0.0625 g, 0.573 mmol) was added to an aqueous solution (10 ml) containing $Zn(ClO_4)_2·6H_2O$ (0.1035 g, 0.278 mmol) and NaI (0.0870 g, 0.580 mmol). Colourless crystals of (I) were obtained after the solution was allowed to stand at room temperature for three weeks.

Crystal data

$[Zn(I)_2(C_6H_7NO)_2]$
M_r = 537.42
Monoclinic, $C2/c$
a = 19.385 (5) Å
b = 7.5134 (19) Å
c = 14.859 (4) Å
β = 126.487 (3)°
V = 1739.9 (8) Å^3
Z = 4
D_x = 2.052 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1828 reflections
θ = 2.6–26.0°
μ = 4.96 mm^{-1}
T = 293 (2) K
Prism, colourless
0.21 × 0.12 × 0.09 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.406, T_{max} = 0.637
4279 measured reflections
1597 independent reflections
1371 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.5°
$h = -23 \rightarrow 20$
$k = -9 \rightarrow 8$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.037P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.59$ e Å^{-3}
1597 reflections	$\Delta\rho_{min} = -0.49$ e Å^{-3}
88 parameters	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.992 (3)	Zn1—I1	2.5399 (6)
O1—Zn1—O1^{i}	102.7 (2)	O1—Zn1—I1^{i}	108.00 (9)
O1—Zn1—I1	108.34 (9)	I1—Zn1—I1^{i}	120.11 (3)

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

All H atoms were placed in calculated positions and included in the final cycles of refinement using a riding model (C—H = 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms); U_{iso}(H) = $1.2U_{eq}$(C) for aromatic H atoms and $1.5U_{eq}$(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* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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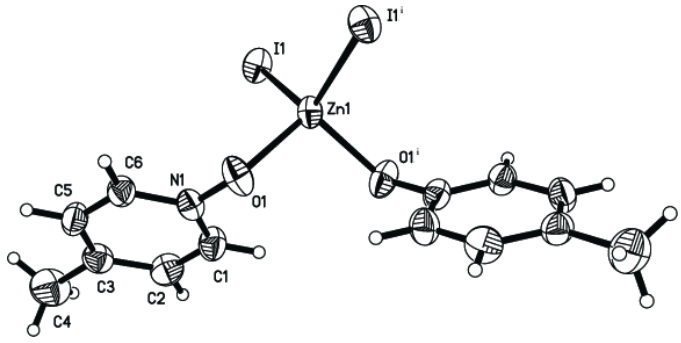

Figure 1
A view of complex (I), with the atom-numbering scheme, showing 30% probability displacement ellipsoids [symmetry code: (i) $1-x, y, \frac{3}{2}-z$]. H atoms are shown as small spheres of arbitary radii.

References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5. A06). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.