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[3,5-Dibromosalicylaldehyde (2-hydroxybenzoyl)-hydrazonato-κ^3O,N,O']bis(pyridine-κN)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.012 Å
R factor = 0.052
wR factor = 0.157
Data-to-parameter ratio = 15.4

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

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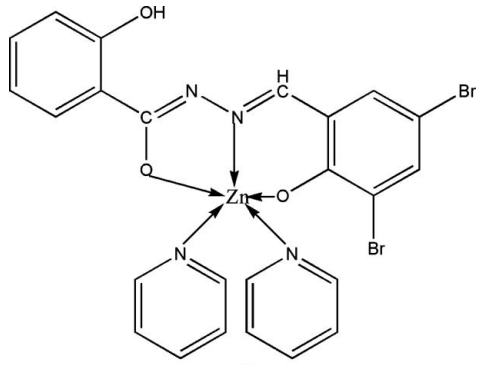
In the title compound, $[Zn(C_{14}H_8Br_2N_2O_3)(C_5H_5N)_2]$, the Zn^{II} ion is coordinated by one N and two O atoms from a Schiff base ligand and by the N atoms of two pyridine molecules to form a distorted trigonal–bipyramidal geometry.

Comment

Previously, we have reported the crystal structure and properties of a 3,5-dibromosalicylaldehyde salicylhydrazone zinc(II) complex (Hu *et al.*, 2005). We now report the synthesis and crystal structure of the title compound, (I).



(I)

The Zn^{II} ion is coordinated by one N and two O atoms from the 3,5-dibromosalicylaldehyde salicylhydrazone ligand, and

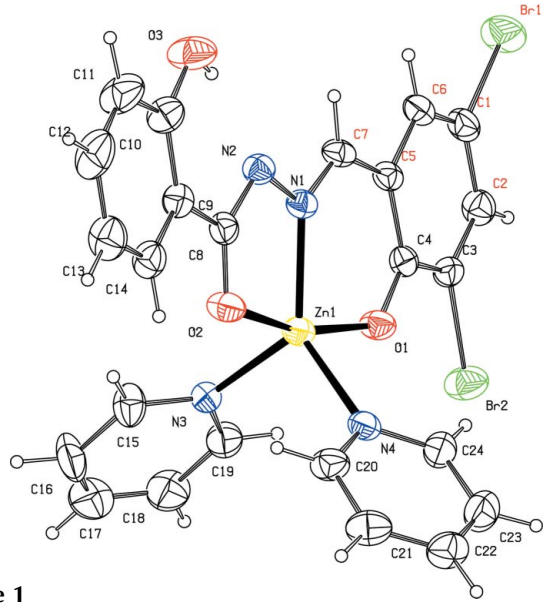


Figure 1
A view of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

by two N atoms of two pyridine molecules (Fig. 1). This ZnN_3O_2 coordination forms a distorted trigonal–bipyramidal geometry (Table 1). Intramolecular O—H···N and C—H···O hydrogen bonds are observed in the Schiff base ligand (Table 2).

Experimental

To an ethanol solution (100 ml) of salicylhydrazine (6 g), one molar equivalent of 3,5-dibromosalicylaldehyde in ethanol (50 ml) was added slowly with continuous stirring and 3,5-dibromosalicylaldehyde salicylhydrazone precipitated immediately. 3,5-Dibromosalicylaldehyde salicylhydrazone (1 mmol), $Zn(OAc)_2$ (1 mmol), dimethylformamide (30 ml) and pyridine (10 ml) were refluxed for 1 h. The hot solution was filtered and allowed to stand at room temperature for 21 d, whereupon green crystals of (I) were obtained.

Crystal data

$[Zn(C_{14}H_8Br_2N_2O_3)(C_5H_5N)_2]$
M_r = 635.61
Triclinic, $P\overline{1}$
a = 8.9000 (11) Å
b = 12.2172 (14) Å
c = 13.1342 (16) Å
α = 101.696 (2)°
β = 103.519 (2)°
γ = 110.744 (2)°
V = 1232.9 (3) Å^3
Z = 2
D_x = 1.712 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1568 reflections
θ = 2.5–21.0°
μ = 4.27 mm^{-1}
T = 292 (2) K
Block, green
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6745 measured reflections
4740 independent reflections
2763 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°
$h = -10 \rightarrow 9$
$k = -12 \rightarrow 15$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.157
S = 1.01
4740 reflections
308 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.5653P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.976 (4)	Zn1—N4	2.074 (5)
Zn1—N1	2.032 (4)	Zn1—O2	2.077 (4)
Zn1—N3	2.057 (5)		
O1—Zn1—N1	89.04 (17)	N3—Zn1—N4	102.42 (17)
O1—Zn1—N3	96.67 (18)	O1—Zn1—O2	165.38 (15)
N1—Zn1—N3	123.88 (17)	N1—Zn1—O2	77.01 (17)
O1—Zn1—N4	94.43 (19)	N3—Zn1—O2	94.78 (18)
N1—Zn1—N4	132.84 (17)	N4—Zn1—O2	91.95 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24···O1	0.93	2.53	3.073 (8)	118
C20—H20···O2	0.93	2.46	3.022 (8)	119
C19—H19···O1	0.93	2.56	3.108 (8)	118
C15—H15···O2	0.93	2.55	3.110 (8)	119
C14—H14···O2	0.93	2.46	2.779 (8)	100
O3—H3···N2	0.82	1.87	2.582 (6)	145

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with O—H = 0.82 Å, C—H = 0.93 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C,O).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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