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Bis[2-hydroxy-*N*′-(2-methoxybenzylidene)-benzohydrazidato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.105
Data-to-parameter ratio = 15.2

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

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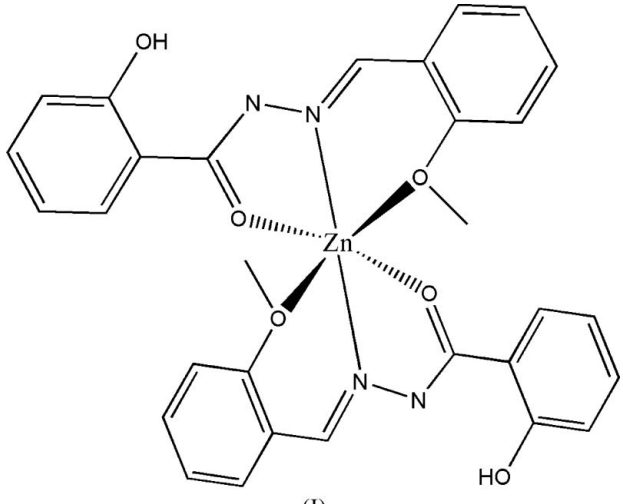
The title compound, $[Zn(C_{15}H_{13}N_2O_3)_2]$, is a mononuclear zinc(II) complex with the metal atom, lying on a twofold rotation axis, coordinated by four O atoms and two N atoms from two anionic 2-hydroxy-*N*′-(2-methoxybenzylidene)benzohydrazide ligands, forming a distorted octahedral coordination configuration.

Comment

Transition metal compounds are present in the active sites of several important classes of metalloproteins. Studies of Schiff base compounds are of great interest in various aspects of chemistry, such as antimicrobial drugs, functional coordinated complexes, photoelectric materials, catalytic materials, *etc.* (Downing & Urbach, 1969; Ganeshpure *et al.*, 1996; Bosnich, 1968; Costes *et al.*, 1995; Duda *et al.*, 2003). The crystal structures of zinc(II) complexes have been widely studied (Howard *et al.*, 2006; Granifo *et al.*, 2006; Tong, 2005; You, 2005*a*,*b*). As an extension of the work on the structural characterization of Schiff base complexes, the preparation and crystal structure of the title Schiff base zinc(II) complex, (I), are reported here.



(I)

The molecular structure of (I), a mononuclear zinc(II) complex, is illustrated in Fig. 1. Selected bond distances and angles are given in Table 1. The Zn^{II} atom, which lies on an symmetry center, has a octahedral geometry and is six-coordinated by four O atoms and two N atoms from two anionic 2-hydroxy-*N*′-(2-methoxybenzylidene)benzohydrazide ligands. The angle for equatorial donor atoms [79.96 (8)° for N2—Zn—O2] correlates with the strained ligand bite angle for the

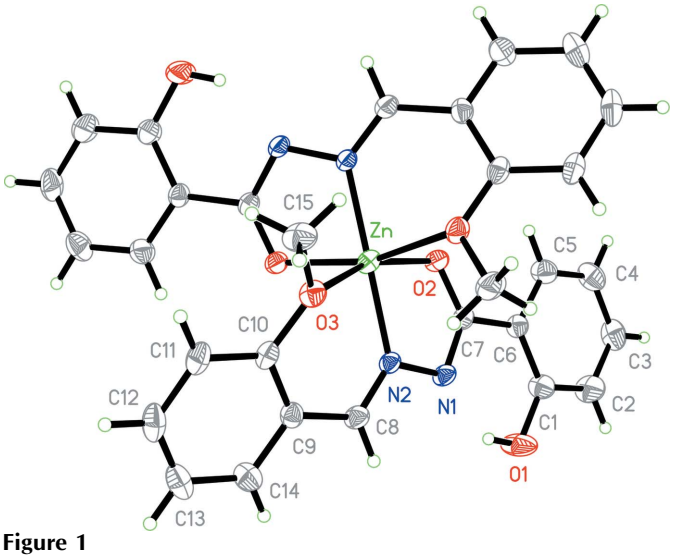


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry operation $(y, x, -z)$.

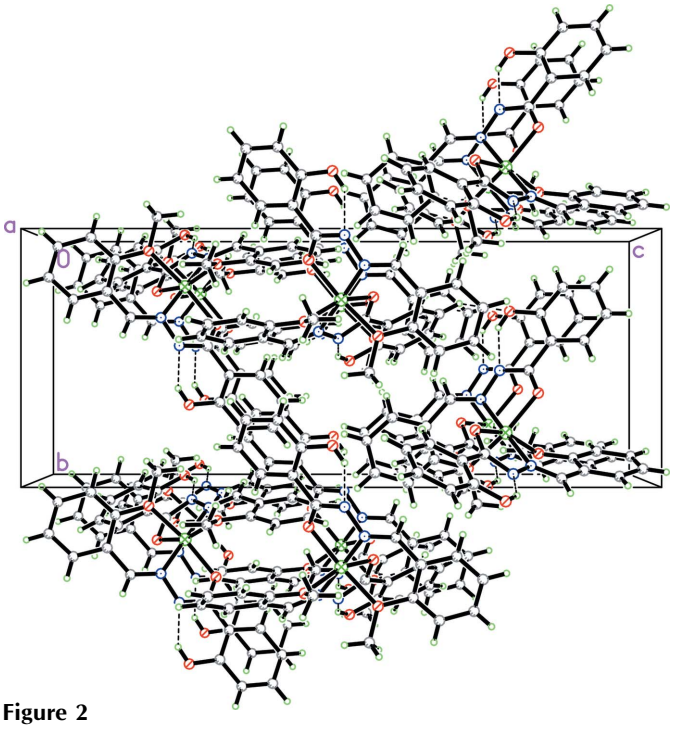


Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

five-membered chelate ring Zn—O2—C7—N1—N2, and the angle for N2—Zn—O3 [83.56 (8)°] correlates loosely with the six-membered ring Zn—O2—C8—C9—C10—O3. The other equatorial angles are closer to 90° [range from 83.90 (11) to 106.70 (11)°]. The *trans* angle $N2^{i}$—Zn—N2 (symmetry code as in Table 1) at the zinc(II) center is close to 180° [177.68 (13)°], but the angle O2—Zn—O3 [159.88 (7)°] deviates significantly from the ideal 180°. The dihedral angle between the two bezene rings of the Schiff base ligand is 23.5 (3)°.

In the crystal structure, the molecules stack along the *a* axis with no short contacts except for the intramolecular hydrogen bond (O1—H1···N1) (Table 2 and Fig. 2).

Experimental

All chemicals were obtained from commercial sources and were used without purification. 2-Hydroxybenzohydrazide (30.4 mg, 0.2 mmol) and 2-methoxybenzaldehyde (27.2 mg, 0.2 mmol) were dissolved in anhydrous methanol (20 ml). The mixture was stirred for 30 min at room temperature to give a clear yellow solution. To this solution was added a methanol solution (10 ml) of $Zn(OAc)_2$ (0.1 mmol, 18.4 mg) with stirring. The resulting solution was allowed to stand in air for 11 d, after which time colorless block-shaped crystals of (I) formed at the bottom of the vessel on slow evaporation of the methanol.

Crystal data

$[Zn(C_{15}H_{13}N_2O_3)_2]$
M_r = 603.92
Tetragonal, $P4_12_12$
a = 10.3578 (6) Å
c = 25.651 (3) Å
V = 2752.0 (4) Å^3
Z = 4
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 295 (2) K
Block, colorless
0.41 × 0.18 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.798, T_{max} = 0.864
22149 measured reflections
2853 independent reflections
2737 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.14
2853 reflections
188 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1128 Freidel pairs
Flack parameter: 0.083 (15)

Table 1
Selected geometric parameters (Å, °).

Zn—N2	1.987 (2)	Zn—O3	2.191 (2)
Zn—O2	2.009 (2)		
$N2^{i}$—Zn—N2	177.68 (13)	O2—Zn—$O3^{i}$	87.07 (8)
N2—Zn—$O2^{i}$	98.63 (8)	N2—Zn—O3	83.56 (8)
N2—Zn—O2	79.96 (8)	O2—Zn—O3	159.88 (7)
$O2^{i}$—Zn—O2	106.70 (11)	$O3^{i}$—Zn—O3	83.90 (11)
N2—Zn—$O3^{i}$	98.18 (8)		

Symmetry code: (i) $y, x, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.86	2.572 (3)	145

All H atoms were positioned geometrically (O—H = 0.82 Å and C—H = 0.93 or 0.96 Å) and constrained to ride on their parent atoms

with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms or $1.5U_{eq}$(methyl C and hydroxyl O).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2002); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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