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Bis[2-(2-oxidophenyl)-1*H*-benzimidazole-κ^2N^3,O]zinc(II) dimethylformamide disolvate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.069
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.

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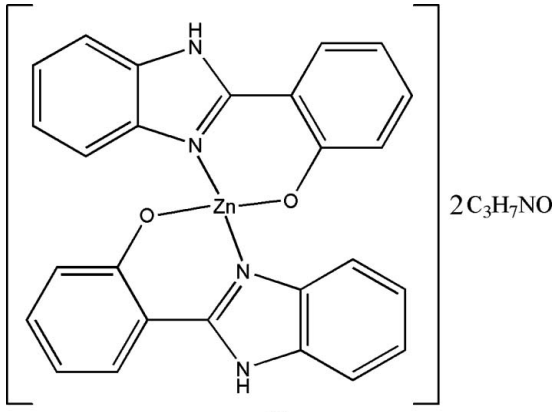
In the title compound, $[Zn(C_{13}H_9N_2O)_2]\cdot 2C_3H_7NO$, the Zn^{II} ion is located on a twofold axis and chelated by two 2-(2-hydroxyphenyl)benzimidazole ligands with a distorted tetrahedral geometry.

Comment

2-(2-Hydroxyphenyl)benzimidazole (Hbzim) complexes have shown potential applications in the fabrication of organic electroluminescent devices. Several complexes incorporating Hbzim have been reported previously (Tong & Li, 2004; Tong *et al.*, 2005; Bu *et al.*, 2005; Xi *et al.*, 2005). Recently, we prepared the new title complex, (I), with the Hbzim ligand, and determined its crystal structure.



(I)

The molecular structure of (I) is shown in Fig. 1. The Zn^{II} ion is located on a twofold axis and is chelated by two planar, deprotonated 2-(2-hydroxyphenyl)benzimidazole ligands in a distorted tetrahedral coordination geometry. The dihedral angle between the two ligand planes is 80.0 (2)°. The bond angles at Zn1 range from 94.48 (5) to 125.70 (7)°, indicating considerable distortion from a normal tetrahedron (Table 1).

The solvent dimethylformamide (DMF) molecules link with the complex *via* N—H···O hydrogen bonding (Fig. 1 and Table 2).

Experimental

2-(2-Hydroxyphenyl)benzimidazole was synthesized according to the procedure reported by Addison & Burke (1981). An ethanol solution (15 ml) of zinc acetate dihydrate (0.11 g, 0.5 mmol), 2-(2-hydroxyphenyl)benzimidazole (0.21 g, 1 mmol) and sodium hydroxide (0.04 g, 1 mmol) was refluxed for 2 h. The resulting white precipitate was filtered off, dried and then dissolved in DMF. Colorless single crystals of (I) were obtained after one month.

Crystal data

$[Zn(C_{13}H_9N_2O)_2]\cdot 2C_3H_7NO$
M_r = 630.01
Orthorhombic, *Pbcn*
a = 15.4137 (11) Å
b = 8.7799 (6) Å
c = 22.0554 (15) Å
V = 2984.8 (4) Å^3
Z = 4
D_x = 1.402 Mg m^{-3}
Mo *Kα* radiation
μ = 0.87 mm^{-1}
T = 293 (2) K
Block, colorless
0.33 × 0.23 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.762, T_{max} = 0.838
17219 measured reflections
3562 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.00
3562 reflections
197 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.9171 (11)	Zn1—N1	1.9721 (12)
O1—Zn1—O1^{i}	125.70 (7)	O1—Zn1—N1	94.48 (5)
O1—Zn1—N1^{i}	111.15 (5)	N1^{i}—Zn1—N1	122.52 (7)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O2	0.86	1.94	2.7729 (18)	162

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C,N).

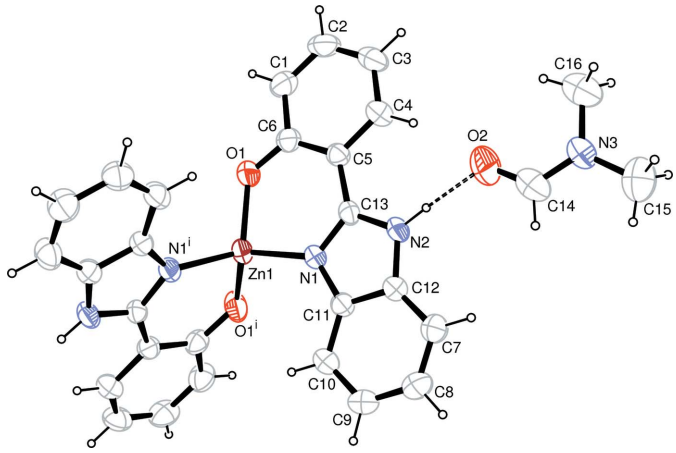


Figure 1
The molecular structure of (I) shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (i) $-x, y, -z+\frac{1}{2}$]. The dashed line indicates the hydrogen bond.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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