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Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(C-C)$ = 0.006 Å
 R factor = 0.064
 wR factor = 0.145
 Data-to-parameter ratio = 16.6

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

Bis{2'-[1-(2-hydroxyphenyl)ethylidene]-benzohydrazido}bis(pyridine- κ N)zinc(II)

In the centrosymmetric title compound, $[Zn(C_{15}H_{13}N_2O_2)_2 \cdot (C_5H_5N)_2]$, the Zn atom is chelated by the O and N atoms of two bidentate ligands. The coordination geometry of the central Zn atom is octahedral. The crystal packing is stabilized by intermolecular C—H...O interactions.

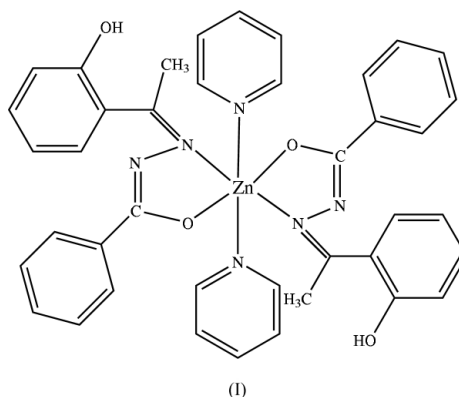
Received 12 May 2004

Accepted 17 May 2004

Online 29 May 2004

Comment

Recrystallization of $[Zn(C_{15}H_{12}N_2O_2)_2]$ from DMSO gives dimeric $[Zn_2(C_{15}H_{12}N_2O_2)_2(C_2H_6OS)_2]$ (Ali *et al.*, 2003). However, the title compound, (I), obtained by recrystallization of the same complex from pyridine, is monomeric and centrosymmetric about the central Zn atom (Fig. 1). The coordination geometry of the Zn atom is octahedral, where atoms N1, N1ⁱ, O2 and O2ⁱ (symmetry code as in Table 1) occupy the equatorial positions, with the *cis* angles lying in the range 76.19 (8)–92.88 (9)°. The bidentate ligands chelate to the Zn atom *via* O and N atoms. Two pyridine groups occupy the axial positions. The basal atoms (Zn1, O2, N1ⁱ, O2ⁱ and N1) are perfectly coplanar. The Zn1–N1 bond length of 2.2222 (10) Å is slightly longer than that in the complex $[Zn_2(C_{15}H_{12}N_2O_2)_2(C_2H_6OS)_2]$, *viz.* 2.0466 (16) Å (Ali *et al.*, 2003). The structural dimensions of the bidentate ligand (Table 1) are in the normal ranges (Allen *et al.*, 1987; Orpen *et al.*, 1989) and comparable with those in the dimeric DMSO complex. The chelate ring Zn1/O2/C9/N2/N1ⁱ is planar, with a maximum deviation from the mean plane of 0.072 (2) Å for atom O2. The benzene ring C9/C10–C15 and the phenol group O1/C1–C6 are each planar and form a dihedral angle of 37.5 (2)°. There are intramolecular O—H...N and C—H...O interactions (Table 2). The crystal packing is stabilized by intermolecular C13—H13A...O1ⁱⁱ interactions (symmetry code as in Table 2), which form zigzag polymeric chains extending along the *b* axis (Fig. 2).



Experimental

The complex was synthesized by the template condensation of 2-hydroxyacetophenonebenzhydrazone (0.3 g, 2.2 mmol) with zinc acetate dihydrate (0.24 g, 1.1 mmol) by refluxing and stirring in ethanol for 5 h. The light-yellow solid was filtered off and recrystallized from pyridine–ethanol.

Crystal data

[Zn(C₁₅H₁₃N₂O₂)₂(C₅H₅N)₂]
M_r = 730.12
 Monoclinic, *P*2₁/*c*
a = 10.3531 (11) Å
b = 15.0133 (16) Å
c = 11.6892 (12) Å
 β = 95.138 (2)°
V = 1809.6 (3) Å³
Z = 2

D_x = 1.340 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2851 reflections
 θ = 1.9–27.0°
 μ = 0.73 mm⁻¹
T = 293 (2) K
 Block, light yellow
 0.29 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.817, *T_{max}* = 0.892
 9919 measured reflections

3933 independent reflections
 3304 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
 θ_{max} = 27.0°
h = -13 → 11
k = -19 → 15
l = -13 → 14

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.064
wR (*F*²) = 0.145
S = 1.22
 3933 reflections
 237 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.6177P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.54 e Å⁻³
 Δρ_{min} = -0.24 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1–O2 ⁱ	2.0261 (19)	O2–C9	1.267 (3)
Zn1–N3 ⁱ	2.222 (3)	N1–C7	1.284 (4)
Zn1–N1 ⁱ	2.223 (2)	N1–N2 ⁱ	1.395 (3)
O1–C5	1.351 (5)	N2–C9	1.312 (4)
O2 ⁱ –Zn1–O2	180	O2–Zn1–N1	103.81 (8)
O2–Zn1–N3 ⁱ	90.56 (9)	N3 ⁱ –Zn1–N1	92.88 (9)
O2–Zn1–N3	89.44 (9)	N3–Zn1–N1	87.12 (9)
N3 ⁱ –Zn1–N3	180	N1–Zn1–N1 ⁱ	180
O2 ⁱ –Zn1–N1	76.19 (8)		

Symmetry code: (i) 2 - *x*, -*y*, 1 - *z*.

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1O···N1	0.77 (4)	2.56 (4)	3.120 (4)	131 (3)
O1–H1O···N2 ⁱ	0.77 (4)	1.83 (4)	2.545 (4)	155 (3)
C8–H8A···O2	0.96	2.24	3.185 (4)	167
C13–H13A···O1 ⁱⁱ	0.93	2.50	3.344 (5)	152

Symmetry codes: (i) 2 - *x*, -*y*, 1 - *z*; (ii) 1 + *x*, $\frac{1}{2}$ - *y*, $\frac{1}{2}$ + *z*.

After their location in a difference map, all H atoms except those on atom O1 were positioned geometrically and allowed to ride on the parent C atom, with C–H = 0.93–0.96 Å with *U*_{iso}(H) = 1.2 or

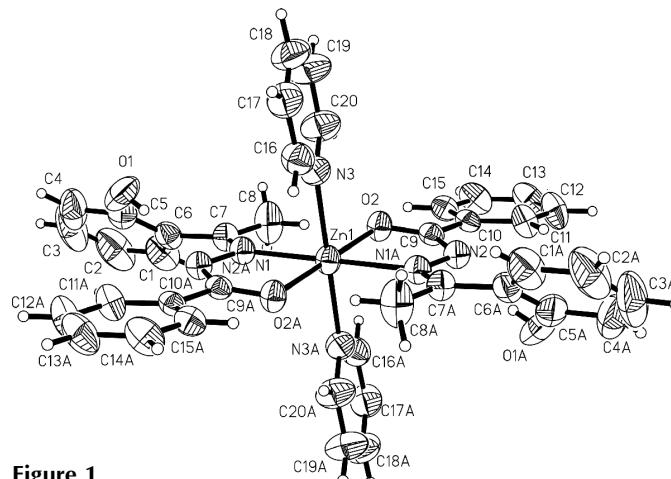


Figure 1

The molecular structure of the title compound, (I), with 50% probability displacement ellipsoids. The suffix *A* corresponds to symmetry code (i) in Table 1.

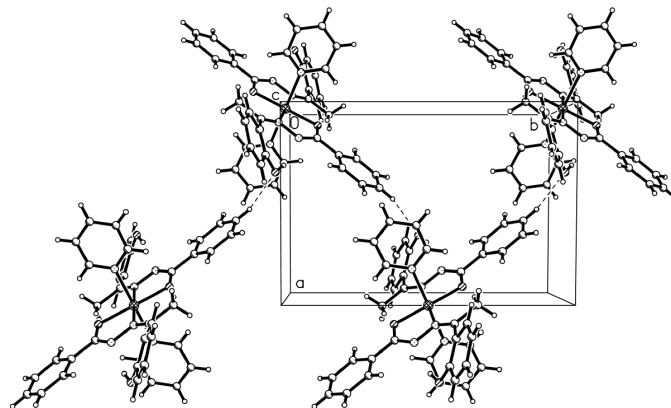


Figure 2

Packing diagram of the title complex, viewed down the *c* axis. Dashed lines denote C–H···O hydrogen bonds.

1.5*U*_{eq}(C). The H atom on O1 was located in a Fourier difference map and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and both Universiti Malaya and Kebangsaan Malaysia for research grants IRPA Nos. 09-02-03-0125 and 09-02-02-993, respectively.

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