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Bis{μ-*N*-[1-(2-oxidophenyl)ethylidene]benzohydrazido}bis[(dimethylsulfoxide)zinc(**II**)]

Hapipah M. Ali,[a] Zuraini Kadir,[a] M. Sukeri M. Yusof[b] and Bohari M. Yamin[b]*

[a]Department of Chemistry, Universiti Malaya, Kuala Lumpur, Malaysia, and [b]School of Chemical Sciences and Food Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor, Malaysia

Correspondence e-mail:
bohari@pkrisc.cc.ukm.my

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.068
Data-to-parameter ratio = 17.2

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

The title compound, $[Zn_2(C_{15}H_{12}N_2O_2)_2(C_2H_6OS)_2]$, is a centrosymmetric dimer *via* a Zn—O bridge of 2.0038 (13) Å, with a Zn···Zn separation of 3.1370 (13) Å. The geometry of the five-coordinate environment of the Zn atoms is close to trigonal bipyramidal.

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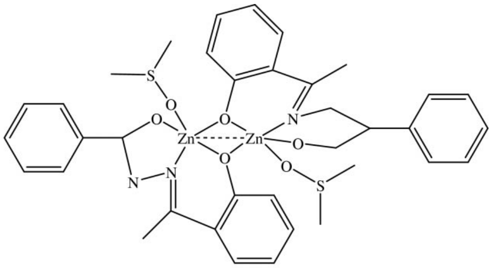
Comment

It is known that recrystallization of some zinc complexes, such as Zn-3,5-diisopropylsalicylate in DMSO, has resulted in the formation of the DMSO derivative $Zn(3,5\text{-DIPS})_2(DMSO)_2$ (Morgant *et al.*, 1998). Similarly, the title compound, (I), was obtained when $[Zn(C_{15}H_{12}N_2O_2)_2]$ was recrystallized from DMSO. However, unlike monomeric $Zn(3,5\text{-DIPS})_2(DMSO)_2$, the crystal structure of (I) (Fig. 1) consists of centrosymmetric dimers, formed by linking two monomeric units through Zn1—O1^{i} and Zn1^{i}—O1 bonds of 2.0038 (13) Å (symmetry code in Table 1). The Zn1···Zn1^{i} separation is 3.1370 (13) Å. The relatively rare five-coordinated zinc complex shows that both central Zn atoms have geometries between square-pyramidal and trigonal bipyramidal, though they are closer to the latter.



(I)

The bond distances and angles (Table 1) are normal (Orpen *et al.*, 1989; Allen *et al.*, 1987). The average Zn—O distance of 2.02 (2) Å is in agreement with the geometry of square pyramidal and trigonal bipyramidal, compared with 1.98 Å for tetrahedral (Morgant *et al.*, 1998) and 2.08 Å for octahedral (Babb *et al.*, 2003). The dimensions of the *O,N,O′*-tridentate ligand are typical of those of a Schiff base. The central Zn1/O1/Zn1^{i}/O1^{i} fragment is planar. The chelating O1/C1/C6/C7/N1 [maximum deviation is 0.045 (2) Å for C6] and O2/C9/N2/N1/C10 fragments are also planar, and inclined by 29.15 (8)° to each other. The two phenyl groups, C1–C6 and C9–C15, make a dihedral angle of 54.64 (8)°.

There is a weak C—H···O intramolecular contact (Table 2). In the crystal structure, the centrosymmetric dimers are linked by intermolecular interactions, C16—H16*C*···O3^{ii}

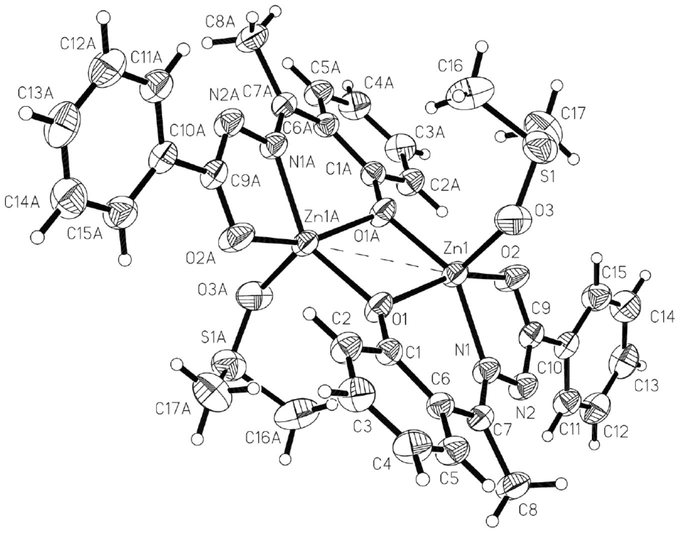


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids. The suffix *A* corresponds to symmetry code (i) in Tables 1 and 2.

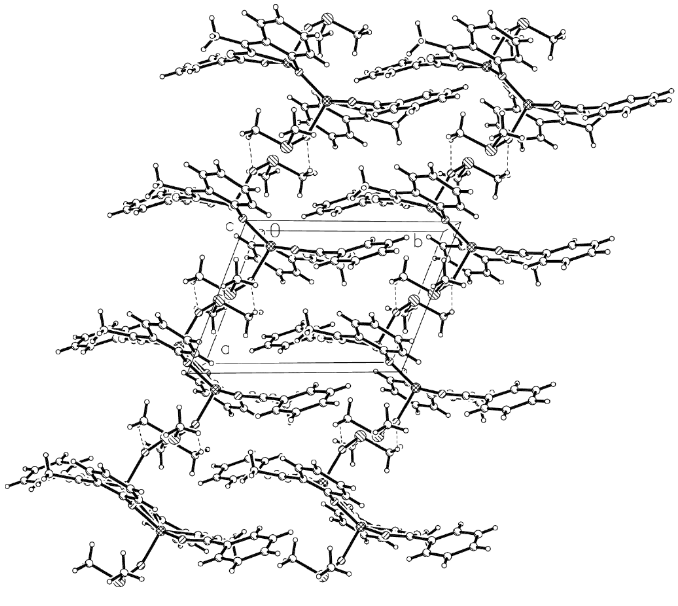


Figure 2
Packing diagram of the title complex, viewed down *c* axis. The dashed lines denote C—H···O intermolecular contacts.

(symmetry code as in Table 2) to form one-dimensional polymeric chains parallel to the *a* axis (Fig. 2).

Experimental

The title complex was synthesized by the template condensation of benzhydrazide (2.00 g, 0.015 mol) and 2-hydroxyacetophenone (2.00 g, 0.015 mol) with zinc acetate dihydrate (1.65 g, 0.007 mol), with refluxing and stirring in ethanol for 5 h in the presence of triethylamine. The resulting pale-yellow solid was filtered and recrystallized from a minimum amount of DMSO. After standing at room temperature for 2 d, pale-yellow crystals were obtained.

Crystal data

$[Zn_2(C_{15}H_{12}N_2O_2)_2(C_2H_6OS)_2]$
$M_r = 791.53$
Triclinic, $P\overline{1}$
$a = 7.690$ (4) Å
$b = 10.214$ (6) Å
$c = 11.643$ (6) Å
$\alpha = 98.479$ (13)°
$\beta = 94.262$ (12)°
$\gamma = 110.338$ (13)°
$V = 840.3$ (8) Å^3
$Z = 1$
$D_x = 1.564$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8764 reflections
$\theta = 1.7$–27.5°
$\mu = 1.60$ mm^{-1}
$T = 293$ (2) K
Block, pale yellow
0.54 × 0.48 × 0.33 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.454$, $T_{\max} = 0.588$
10556 measured reflections
3804 independent reflections
3653 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.068$
$S = 1.10$
3804 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.2073P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0148 (15)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1$^{\rm i}$	2.0038 (13)	O2—C9	1.2834 (19)
Zn1—O2	2.0117 (14)	O3—S1	1.5142 (14)
Zn1—O3	2.0131 (16)	S1—C16	1.761 (2)
Zn1—N1	2.0466 (16)	S1—C17	1.781 (2)
Zn1—O1	2.0683 (15)	N1—C7	1.294 (2)
Zn1···Zn1$^{\rm i}$	3.1370 (13)	N1—N2	1.3949 (17)
O1—C1	1.3391 (17)	N2—C9	1.309 (2)
O2—Zn1—O1	155.78 (5)	O2—Zn1—N1	78.70 (6)
O1$^{\rm i}$—Zn1—O2	105.70 (6)	O3—Zn1—N1	107.52 (5)
O1$^{\rm i}$—Zn1—O3	103.94 (6)	O1$^{\rm i}$—Zn1—O1	79.24 (5)
O2—Zn1—O3	101.22 (6)	O3—Zn1—O1	100.46 (5)
O1$^{\rm i}$—Zn1—N1	146.72 (5)	N1—Zn1—O1	84.59 (5)

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

Table 2
"C—H···O contacts (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2$^{\rm i}$	0.93	2.33	3.167 (3)	149
C16—H16*C*···O3$^{\rm ii}$	0.96	2.42	3.258 (4)	145

Symmetry codes: (i) $-x, -y, 1 - z$; (ii) $1 - x, -y, 1 - z$.

After their location in a difference map, all H atoms were placed geometrically at ideal positions and allowed to ride on the parent C atoms, with C—H = 0.93–0.96 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm C})$.

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).

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