Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis{2′-[1-(2-hydroxy-5-chlorophenyl)ethylidene]-benzohydrazido-$\kappa^2O,N^{2'}$}bis(pyridine-κN)zinc(II)

Hapipah Ali,[a]* Nur Ashikin Khamis[a] 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: hapipahali@yahoo.com

Received 3 August 2004
Accepted 18 August 2004
Online 28 August 2004

Key indicators

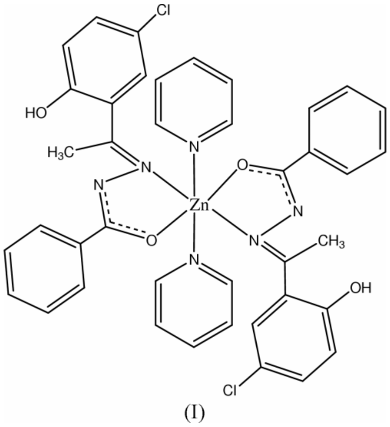
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.134
Data-to-parameter ratio = 16.1

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

The title compound, $[Zn(C_{15}H_{13}ClN_2O_2)_2(C_5H_5N)_2]$, is a centrosymmetric monomer with octahedral geometry about the Zn atom. The molecule is stabilized by intermolecular C—H···O and C—H···Cl interactions, so forming a three-dimensional network.

Comment

Recrystallization of $[Zn(C_{13}H_9ClN_2O_2S)_2]$ from pyridine gave the dimeric compound $[Zn(C_{13}H_9ClN_2O_2S)_2(C_5H_5N)_2]$, with trigonal bipyrimidal geometry at the central Zn atoms (Ali, Mohamad *et al.*, 2004). However, the title compound, $[Zn(C_{15}H_{13}ClN_2O_2)_2](C_5H_5N)_2]$, (I), which was also obtained by recrystallization of $[Zn(C_{15}H_{13}ClN_2O_2)_2]$ from pyridine, is monomeric with an octahedral geometry about the central Zn atom. The complex is also an analogue of the centrosymmetric compound $[Zn(C_{15}H_{13}N_2O_2)_2](C_5H_5N)_2]$ (Ali, Khamis *et al.*, 2004).



(I)

The molecular structure of (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. The ligands are chelated in a bidentate manner *via* atoms O1 and N1, occupying the equatorial positions, the O1—Zn1—N1 bond angle being 103.47 (8)°. The N atoms of the two pyridine molecules occupy the axial positions, the N3—Zn1—N3^i bond angle being 180° [symmetry code: (i) $1 - x$, $-y$, $1 - z$]. The structural dimensions of the ligand are in the normal range (Orpen *et al.*, 1979; Allen *et al.*, 1987) and in agreement with other octahedral zinc complexes (Tesouro Vallina & Stoeckli-Evans, 2002; Ali *et al.*, 2004). The chelated Zn1/O1/C7/N2/N1^i fragment is planar, with a maximum deviation from the mean plane of 0.064 (3) Å for atom N1^i. The C8/C10–C15/O2/Cl1 fragment is planar [maximum deviation at C12 of 0.05 (3) Å] and inclined to the C1–C7 fragment [maximum deviation −0.011 (4) Å for atom C5] by 43.53 (15)°.

DOI: 10.1107/S1600536804020501

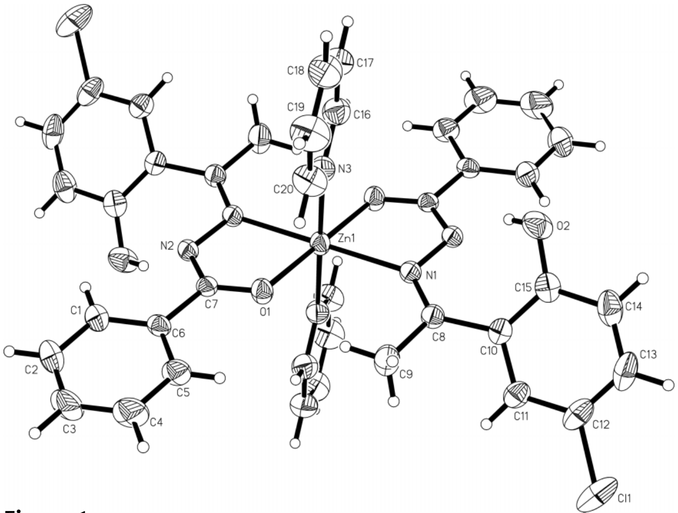


Figure 1
Molecular structure of (I), with 50% probability displacement ellipsoids. H atoms are represented by small spheres.

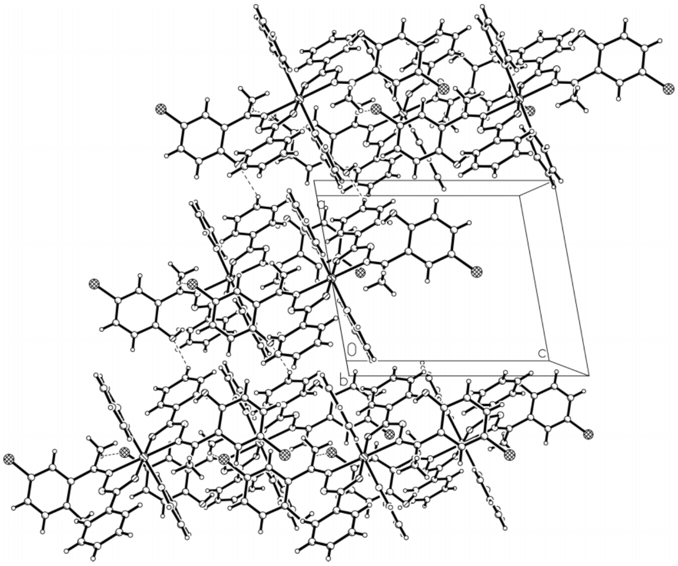


Figure 2
Packing diagram of the title complex, viewed down *b* axis. The dashed lines denote C—H···O and C—H···Cl interactions.

There are important intramolecular hydrogen-bonding interactions in the molecule, and details are given in Table 2. These are interactions of the types O—H···N, involving hydroxyl atom O2 and atom N2, and C—H···O, involving methyl group C9 and carbonyl atom O1 (O2—H2*D*···N2^{i} and C9—H9*A*···O1). In the crystal, the molecules are linked by weak intermolecular C—H···O and C—H···Cl interactions (C3—H3*A*···O2^{ii} and C9—H9*B*···Cl1^{iii}), forming a three-dimensional network, as illustrated in Fig. 2.

Experimental

The complex was synthesized by the template condensation of 2-hydroxy-5-chloroacetophenonebenzhydrazide (0.3 g, 1.0 mmol) with zinc acetate dihydrate (0.11 g, 0.5 mmol), by refluxing and stirring in ethanol for 5 h. The light-yellow solid obtained was filtered off and recrystallized from pyridine.

Crystal data

$[Zn(C_{15}H_{13}ClN_2O_2)_2(C_5H_5N)_2]$
$M_r = 799.00$
Monoclinic, $P2_1/c$
$a = 10.2453$ (17) Å
$b = 15.388$ (3) Å
$c = 12.359$ (2) Å
$\beta = 100.189$ (3)°
$V = 1917.8$ (5) Å^3
$Z = 2$
$D_x = 1.384$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2652 reflections
$\theta = 2.0$–26.5°
$\mu = 0.83$ mm^{-1}
$T = 273$ (2) K
Plate, light yellow
0.48 × 0.46 × 0.09 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.692$, $T_{max} = 0.929$
8429 measured reflections
3939 independent reflections
3205 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.5°$
$h = -9 \rightarrow 12$
$k = -13 \rightarrow 19$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.134$
$S = 1.08$
3939 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.6133P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.022 (2)	N1—C8	1.291 (4)
Zn1—N1	2.206 (2)	N1—N2^{i}	1.393 (3)
Zn1—N3	2.243 (3)	N2—C7	1.321 (4)
Cl1—C12	1.737 (4)	N3—C16	1.324 (5)
O1—C7	1.263 (3)	N3—C20	1.331 (5)
O2—C15	1.348 (5)		
O1^{i}—Zn1—O1	180	O1—Zn1—N3	88.67 (10)
O1^{i}—Zn1—N1	76.53 (8)	N1—Zn1—N3	87.98 (10)
O1—Zn1—N1	103.47 (8)	N1^{i}—Zn1—N3	92.02 (10)
O1^{i}—Zn1—N3	91.33 (10)	N3—Zn1—N3^{i}	180

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O1	0.96	2.24	3.177 (4)	165
O2—H2*D*···N2^{i}	0.87 (5)	1.69 (4)	2.522 (4)	160 (4)
C3—H3*A*···O2^{ii}	0.93	2.47	3.272 (6)	144
C9—H9*B*···Cl1^{iii}	0.96	2.82	3.629 (5)	143

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

All the H atoms could be located from Fourier difference maps. The hydroxyl H atom at O2 was refined isotropically. The remainder were included in calculated positions and treated as riding atoms [C—H$_{ar}$ = 0.93 Å, with U_{iso}(H) = 1.2U_{eq}(C), and C—H$_3$ = 0.96 Å, with U_{iso}(H) = 1.5U_{eq}(C)].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); 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 the research grants IRPA Nos. 09-02-03-0125 and 09-02-02-993, respectively.

References

Ali, H. M., Khamis, N. A., Basirun, W. J. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m873–m875.

Ali, H. M., Mohamad, M., Yusof, M. M. S. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m123–m125.

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1—S3.

Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS*97, *SHELXL*97 and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Tesouro Vallina, A. & Stoeckli-Evans, H. (2002). *Polyhedron*, **21**, 1177–1187.