Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(μ-2,4-dihydroxyacetophenone salicylhydrazidato)bis[pyridinezinc(II)] dimethylformamide disolvate

Jinshan Huang, Yongfei Wu and Xinde Zhu*

Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China

Correspondence e-mail: tzb@mail.ccnu.edu.cn

Received 15 June 2005
Accepted 6 July 2005
Online 13 July 2005

The tridentate Schiff base ligand 2,4-dihydroxyacetophenone salicylhydrazide, derived from the condensation of 2,4-dihydroxyacetophenone and salicylhydrazide, in the presence of pyridine and *N*,*N*′-dimethylformamide, forms a dinuclear distorted square-pyramidal Zn complex with $Zn(OAc)_2 \cdot 2H_2O$, *viz*. $[Zn_2(C_{15}H_{12}N_2O_4)_2(C_5H_5N)_2] \cdot 2C_3H_7NO$. The complex is centrosymmetric and the two Zn atoms are bridged by two phenolate O atoms.

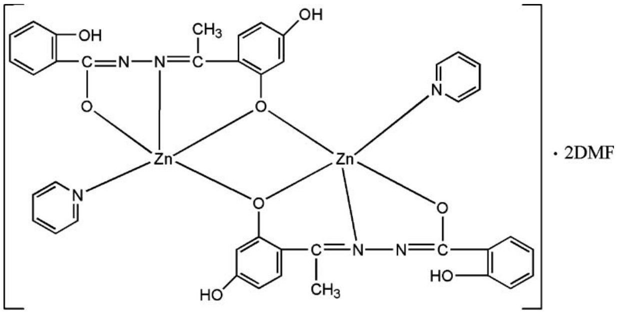
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.140
Data-to-parameter ratio = 14.9

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

Comment

Schiff base compounds have many applications in homogeneous catalysts and antitumor activities (Desai *et al.*, 2001). We report here the synthesis and crystal structure of one such Schiff base complex, namely bis(μ-2,4-dihydroxyacetophenone salicylhydrazidato)bis[pyridinezinc(II)] dimethylformamide disolvate, (I).



(I)

In the crystal structure of (I), there is a centre of symmetry at the mid-point of the Zn···Zn vector (Fig. 1). Each Zn atom has a distorted square-pyramidal coordination geometry, formed by one N atom and two O atoms from one Schiff base ligand, one O atom from another Schiff base ligand, and one N atom from a pyridine molecule. Bond lengths and angles involving Zn1 are listed in Table 1.

The crystal structure is stabilized by hydrogen bonds of the types C—H···O, O—H···O and O—H···N (Table 2 and Fig. 2).

Experimental

To a solution of 2,4-dihydroxyacetophenone salicylhydrazide (0.143 g, 0.5 mmol) in DMF (15 ml), $Zn(OAc)_2 \cdot 2H_2O$ (0.110 g, 0.5 mmol) dissolved in pyridine (5 ml) was added with continuous stirring. The mixture was stirred for 5 h at 323 K. After filtration, the yellow solution was allowed to stand at room temperature. Yellow block-shaped crystals were formed by slow evaporation of the solvent at room temperature over a period of 7 d.

Crystal data

$[Zn_2(C_{15}H_{12}N_2O_4)_2(C_5H_5N)_2]\cdot 2C_3H7NO$
$M_r = 1003.66$
Monoclinic, $P2_1/c$
$a = 9.8061$ (7) Å
$b = 9.9171$ (7) Å
$c = 23.7427$ (17) Å
$\beta = 92.545$ (2)°
$V = 2306.7$ (3) Å^3
$Z = 2$
$D_x = 1.445$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2274 reflections
$\theta = 2.2$–21.6°
$\mu = 1.11$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.733$, $T_{max} = 0.809$
12351 measured reflections
4511 independent reflections
3444 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.0°$
$h = -11 \rightarrow 12$
$k = -11 \rightarrow 12$
$l = -29 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.140$
$S = 1.08$
4511 reflections
303 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.014 (2)	Zn1—N3	2.056 (3)
Zn1—O3^i	2.022 (2)	Zn1—N2	2.071 (3)
Zn1—O3	2.023 (2)		
O1—Zn1—O3^i	158.56 (11)	O3—Zn1—N3	107.55 (11)
O1—Zn1—O3	103.14 (10)	O1—Zn1—N2	79.19 (11)
O3^i—Zn1—O3	78.10 (10)	O3^i—Zn1—N2	86.21 (10)
O1—Zn1—N3	98.03 (11)	O3—Zn1—N2	139.67 (11)
O3^i—Zn1—N3	101.98 (12)	N3—Zn1—N2	111.98 (12)

Symmetry code: (i) $-x, -y + 2, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1	0.93	2.39	3.119 (5)	135
O4—H4A···O5^{ii}	0.82	1.87	2.677 (4)	166
O2—H2A···N1	0.82	1.84	2.561 (4)	146

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

The methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H distances of 0.93 Å.

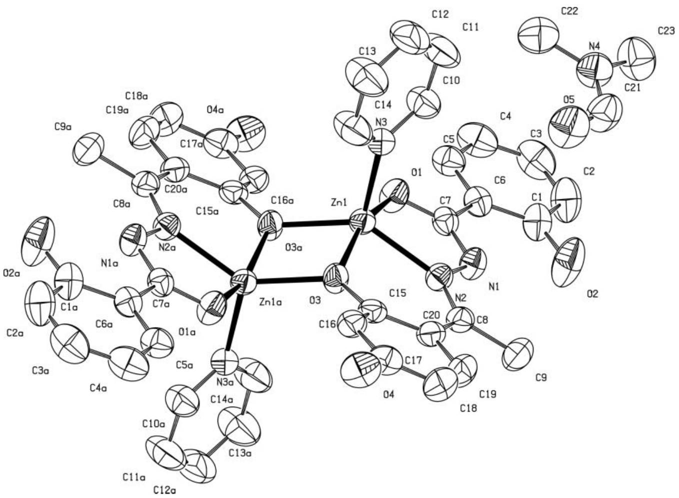


Figure 1
A view of the title complex, showing the labelling of the non-H atoms and 20% probability ellipsoids. The suffix 'a' corresponds to the symmetry position ($-x$, $2 - y$, $-z$). H atoms have been omitted.

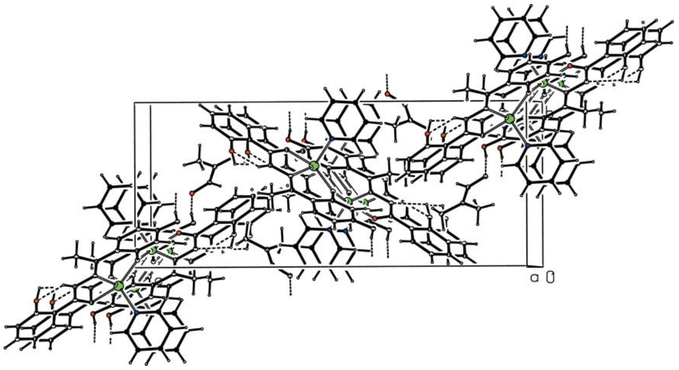


Figure 2
A view of the crystal packing along the *a* axis. Hydrogen bonds are shown as dashed lines.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2001); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2001); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

References

Bruker (2001). *SHELXTL* (Version 6.12), *SADABS* (Version 2.10), *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desai, S. B., Desai, P. B. & Desai, K. R. (2001). *Heterocycl. Commun.* **7**, 83–90.
Sheldrick, G. M. (2001). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Acta Cryst. (2005). E**61**, m1548–m1549 Huang *et al.* • $[Zn_2(C_{15}H_{12}N_2O_4)_2(C_5H_5N)_2]\cdot 2C_3H7NO$ **m1549**