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Bis[2-(cyclopropyliminomethyl)-4-nitrophenolato]zinc(II)

Zhong-Lu You

Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail: youzhonglu@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.120
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.

In the title compound, $[Zn(C_{10}H_9N_2O_3)_2]$, the Zn^{II} centre displays a distorted tetrahedral configuration defined by two imine N and two phenolate O atoms from two Schiff base ligands.

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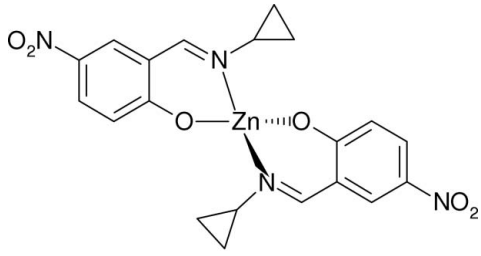
Comment

The crystal structures of a few Schiff base zinc(II) compounds have been previously reported (You, 2005*a*,*b*,*c*). As an extension of the work on these compounds, the title zinc(II) compound, (I), is reported here.



(I)

The bond lengths and angles in (I), a mononuclear zinc(II) compound (Fig. 1), are comparable to those reported for bis[2-(cyclopropyliminomethyl)phenolato]zinc(II) (You *et al.*, 2003). The central Zn^{II} atom is four-coordinate and is bound by two imine N and two phenolate O atoms from two Schiff base ligands. This ZnN_2O_2 centre has a distorted tetrahedral geometry, with angles subtended at the Zn^{II} atom in the range 96.65 (9)–118.69 (10)° (Table 1). In the crystal structure, weak C—H···O interactions are observed (Table 2).

Experimental

Cyclopropylamine and 5-nitrosalicylaldehyde were available commercially and were used without further purification. Cyclo-

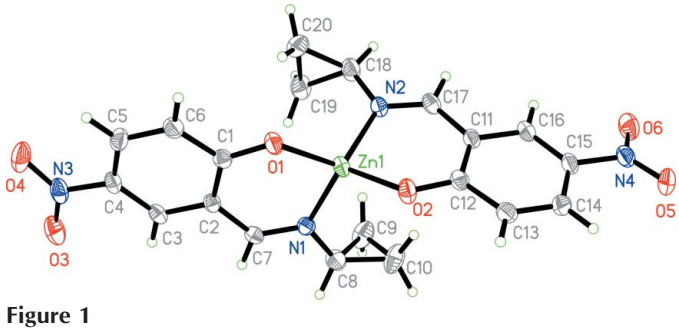


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

propylamine (0.1 mmol, 5.7 mg) and 5-nitrosalicylaldehyde (0.1 mmol, 16.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added a MeOH solution (5 ml) of $Zn(CH_3COO)_2{\cdot}4H_2O$ (0.1 mmol, 25.6 mg), with stirring. The resulting mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 3 d, colourless plate-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[Zn(C_{10}H_9N_2O_3)_2]$
M_r = 475.75
Monoclinic, $P2_1/c$
a = 11.363 (1) Å
b = 16.873 (2) Å
c = 11.266 (1) Å
β = 113.283 (1)°
V = 1984.1 (3) Å^3
Z = 4
D_x = 1.593 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3240 reflections
θ = 2.3–24.2°
μ = 1.29 mm^{-1}
T = 298 (2) K
Plate, colourless
0.18 × 0.13 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.802, T_{max} = 0.915
16852 measured reflections
4519 independent reflections
3579 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.5°
$h = -14 \rightarrow 14$
$k = -21 \rightarrow 21$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.120
S = 1.08
4519 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.5393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.908 (2)	Zn1—N2	2.010 (3)
Zn1—O2	1.909 (2)	Zn1—N1	2.019 (3)
O1—Zn1—O2	118.69 (10)	O1—Zn1—N1	96.65 (9)
O1—Zn1—N2	115.15 (10)	O2—Zn1—N1	114.47 (11)
O2—Zn1—N2	96.93 (10)	N2—Zn1—N1	116.33 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O4^{i}	0.93	2.59	3.366 (4)	142
C17—H17···O3^{ii}	0.93	2.44	3.349 (5)	165
C20—H20A···O1	0.97	2.58	3.398 (4)	142

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $x-1, y, z-1$.

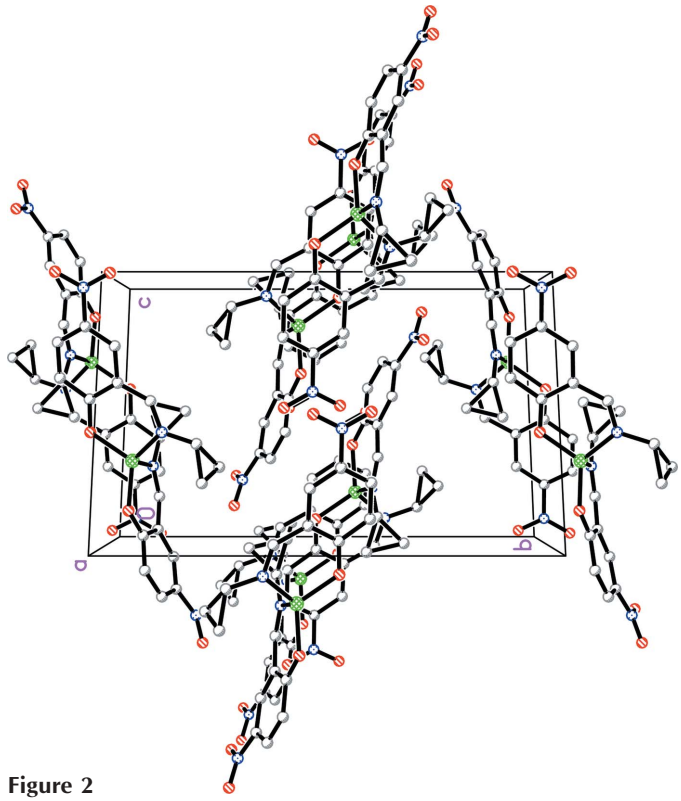


Figure 2
The crystal packing of (I), viewed along the a axis. H atoms have been omitted.

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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