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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.108
Data-to-parameter ratio = 17.4

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

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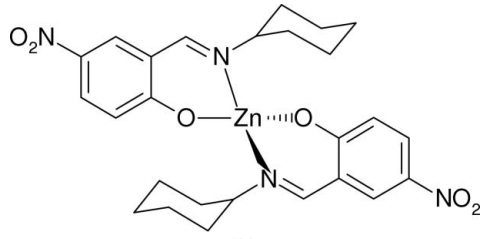
In the mononuclear title compound, $[Zn(C_{13}H_{15}N_2O_3)_2]$, the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two imine N and two phenolate O atoms from two Schiff base ligands.

Comment

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



(I)

Complex (I), a mononuclear zinc(II) compound (Fig. 1), is structurally similar to bis[2-(cyclopropyliminomethyl)phenolato]zinc(II), [(II); You *et al.*, 2003]. The bond lengths and angles (Table 1) in (I) are comparable to those in (II). The central Zn^{II} atom is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligands. This ZnN_2O_2 coordination forms a distorted tetrahedral geometry, with angles subtended at the Zn^{II} atom in the range 96.25 (7)–123.95 (8)°. In the crystal structure, centrosymmetrically related molecules are linked through C—H···O hydrogen bonds (Table 2) and C—H···π interactions involving the C1–C6 benzene ring (centroid *Cg*1).

Experimental

Cyclohexylamine (0.1 mmol, 9.9 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 11 d, colourless block-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[Zn(C_{13}H_{15}N_2O_3)_2]$
M_r = 559.91
Triclinic, $P\overline{1}$
a = 10.759 (1) Å
b = 11.108 (1) Å
c = 12.439 (1) Å
α = 113.74 (1)°
β = 104.39 (1)°
γ = 94.99 (1)°
V = 1288.5 (2) Å^3
Z = 2
D_x = 1.443 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4267 reflections
θ = 2.3–25.5°
μ = 1.00 mm^{-1}
T = 298 (2) K
Block, colourless
0.21 × 0.12 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.817, T_{max} = 0.898
14907 measured reflections
5819 independent reflections
4828 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.108
S = 1.09
5819 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.1392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.918 (2)	Zn1—N1	1.998 (2)
Zn1—O1	1.927 (2)	Zn1—N2	2.000 (2)
O2—Zn1—O1	119.44 (8)	O2—Zn1—N2	96.40 (7)
O2—Zn1—N1	112.74 (8)	O1—Zn1—N2	109.86 (8)
O1—Zn1—N1	96.25 (7)	N1—Zn1—N2	123.95 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O3^{i}	0.98	2.43	3.380 (3)	163
C24—H24B···$Cg1^{ii}$	0.97	2.78	3.680 (4)	155

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$. Note: $Cg1$ is the centroid of the C1–C6 benzene ring.

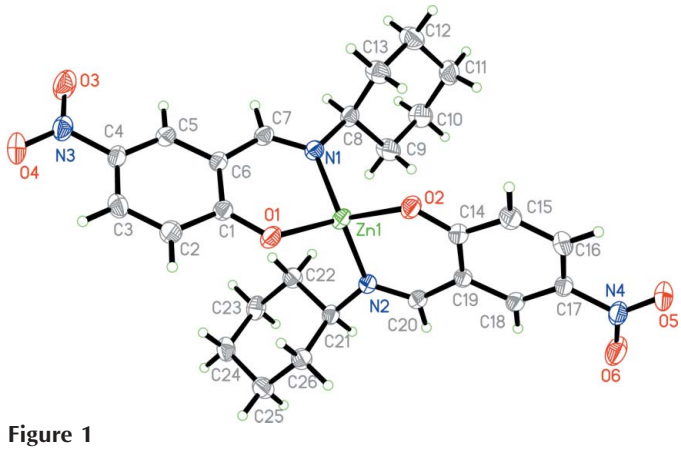


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 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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