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Azido{2,4-dichloro-6-[2-(diethylamino)-ethyliminomethyl]phenolato}zinc(II)

Qing Wang

Office of Organization, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China

Correspondence e-mail: wangqing_fy@126.com

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The Zn^{II} atom in the title mononuclear zinc(II) complex, $[Zn(C_{13}H_{17}Cl_2N_2O)(N_3)]$, is four-coordinated in a distorted square-planar geometry by one Schiff base ligand and one azide anion.

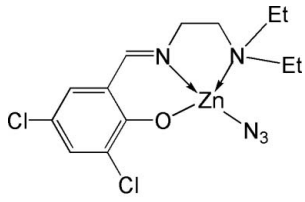
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.105
Data-to-parameter ratio = 15.8

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

Comment

As a continuation of our work on the crystal structures of Schiff base complexes (Wang & Fang, 2006*a*,*b*), the crystal structure of the title mononuclear zinc(II) complex, (I), is reported in this paper.



(I)

The Zn^{II} ion in (I) is four-coordinated by one O atom, one imine N atom and one amine N atom of the Schiff base ligand, and by one N atom of an azide anion, forming a distorted square-planar geometry, as shown in Fig. 1. The geometric parameters around the Zn1 centre (Table 1) are comparable with the values observed in other similar zinc(II) complexes (Yang, 2005; Ju *et al.*, 2005; Odoko *et al.*, 2006; Choi *et al.*, 2005).

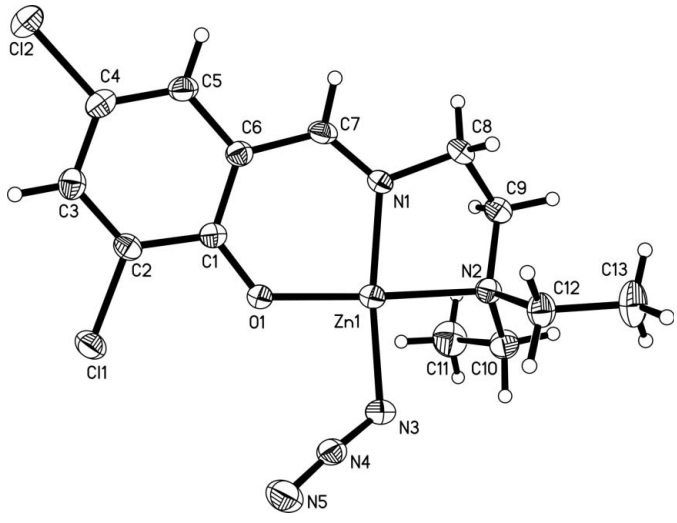


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

3,5-Dichloro-2-hydroxybenzaldehyde (1.0 mmol, 291.0 mg), *N*,*N*-dimethylethane-1,2-diamine (1.0 mmol, 88.2 mg), sodium azide (1.0 mmol, 65.0 mg) and $Zn(NO_3)_2{\cdot}6H_2O$ (1.0 mmol, 297.5 mg) were dissolved in an EtOH/H_2O (100 ml, 5:1 *v*/*v*) solution. The mixture was stirred for 30 min at room temperature to give a colourless solution. X-ray diffraction quality crystals were formed by evaporation of the solvents in an open atmosphere over a period of several days.

Crystal data

$[Zn(C_{13}H_{17}Cl_2N_2O)(N_3)]$
M_r = 395.59
Monoclinic, $P2_1/c$
a = 10.755 (1) Å
b = 11.544 (1) Å
c = 13.229 (1) Å
β = 99.31 (2)°
V = 1620.8 (3) Å^3
Z = 4
D_x = 1.621 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.85 mm^{-1}
T = 293 (2) K
Block, colourless
0.45 × 0.41 × 0.37 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.489, T_{max} = 0.547
(expected range = 0.450–0.504)
12003 measured reflections
3180 independent reflections
2727 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.05
3180 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.7826P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.898 (2)	Zn1—N3	1.953 (2)
Zn1—N1	1.941 (2)	Zn1—N2	2.074 (2)
O1—Zn1—N1	93.60 (9)	O1—Zn1—N2	171.21 (9)
O1—Zn1—N3	92.68 (10)	N1—Zn1—N2	84.41 (10)
N1—Zn1—N3	164.36 (11)	N3—Zn1—N2	91.43 (10)

H atoms attached to the C atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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