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Nitrato[1-(2-pyridylmethyliminomethyl)-naphthalen-2-olato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.0052 Å
R factor = 0.039
wR factor = 0.114
Data-to-parameter ratio = 14.2

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

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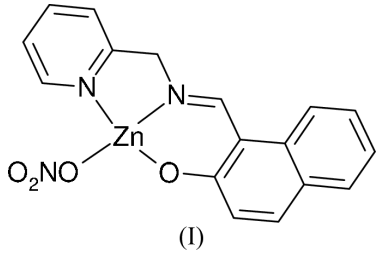
In the title mononuclear zinc(II) compound, [Zn($C_{17}H_{13}N_2O$)(NO_3)], the Zn atom is four-coordinate, bonded to two N atoms and one O atom from the Schiff base ligand, and to one O atom from the nitrate anion. The four atoms around the Zn atom adopt an approximately square-planar configuration.

Comment

Transition metal compounds containing Schiff base ligands have been of interest for a long time (Archer & Wang, 1990; Chang *et al.*, 1998). These compounds play an important role in the development of coordination chemistry (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Zinc has long been recognized as an important cofactor in biological molecules (Vallee & Auld, 1993; Lipscomb & Sträter, 1996; Matthews & Goulding, 1997; Wilker & Lippard, 1997). As an extension of work on the structural characterization of Schiff base–Zn^{II} complexes, the structure of the title compound, (I), is reported here.



(I)

In the molecule of (I), the Zn^{II} atom is four-coordinate, bonded to one O and two N atoms from the Schiff base ligand, and to one O atom from the coordinated nitrate anion (Fig. 1).

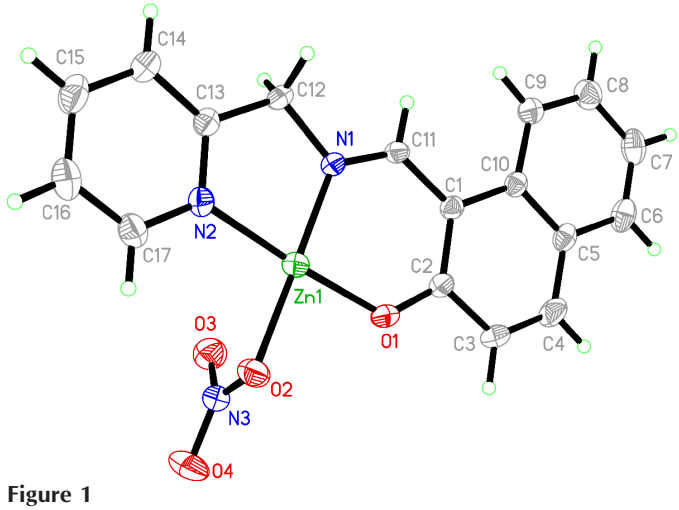


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

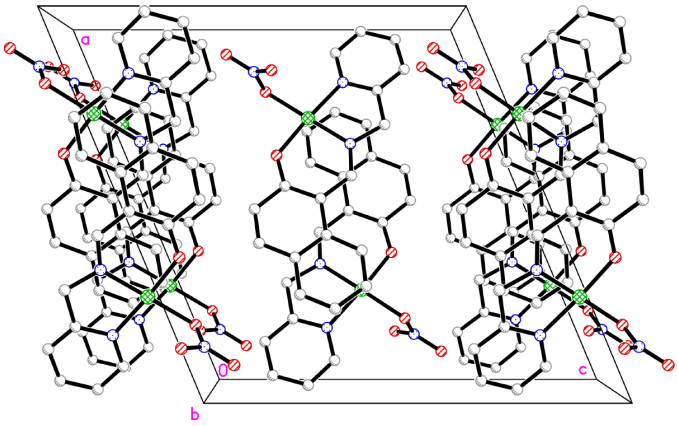


Figure 2
The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted.

The four coordinating atoms around the Zn atom are approximately coplanar, giving a square-planar configuration with an average deviation of 0.004 (3) Å; the Zn atom lies 0.036 (2) Å above this plane. The Zn1—O1 bond [1.880 (2) Å] is a little shorter than the value observed in another Schiff base–Zn complex, aqua[2-(pyridin-2-ylmethyliminomethyl)-phenolato]zinc(II) nitrate monohydrate, (II) [1.892 (2) Å; Li & Zhang, 2004]. The Zn1—N1 bond [1.913 (2) Å] is also a little shorter than the value observed in (II) [1.927 (2) Å]. The Zn1—N2 and Zn1—O2 bond lengths are comparable with the values found in (II).

In the crystal structure of (I) (Fig. 2), the molecules stack along the *b* axis with no short (<3.2 Å) molecular contacts.

Experimental

2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg) and 2-amino-methylpyridine (0.2 mmol, 21.7 mg) were dissolved in methanol (15 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 (10 ml) of $Zn(NO_3)\cdot 2H_2O$ (0.2 mmol, 45.1 mg) with stirring. The mixture was stirred for about 20 min at room temperature and filtered. After keeping the filtrate in air for 5 d, yellow block-shaped crystals of (I) were formed on slow evaporation of the solvent. The crystals were isolated, washed three times with MeOH and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 72.9%). Analysis found: C 52.3, H 3.4, N 11.0%; calculated for $C_{17}H_{13}N_3O_4Zn$: C 52.5, H 3.4, N 10.9%.

Crystal data

$[Zn(C_{17}H_{13}N_2O)(NO_3)]$	D_x = 1.664 Mg m^{-3}
M_r = 388.67	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2887 reflections
a = 15.105 (2) Å	θ = 2.7–25.7°
b = 7.398 (2) Å	μ = 1.61 mm^{-1}
c = 15.056 (2) Å	T = 273 (2) K
β = 112.72 (1)°	Block, yellow
V = 1551.9 (5) Å^3	0.22 × 0.21 × 0.17 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	3202 independent reflections
φ and ω scans	2705 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.024
T_{min} = 0.711, T_{max} = 0.764	θ_{max} = 26.5°
8760 measured reflections	$h = -18 \rightarrow 11$
	$k = -9 \rightarrow 9$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.5874P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.114	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
3202 reflections	
226 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.880 (2)	Zn1—O2	2.013 (2)
Zn1—N1	1.913 (2)	N1—C11	1.287 (3)
Zn1—N2	1.981 (2)	N1—C12	1.466 (3)
O1—Zn1—N1	93.06 (9)	O1—Zn1—O2	88.53 (9)
O1—Zn1—N2	176.32 (9)	N1—Zn1—O2	177.16 (9)
N1—Zn1—N2	83.73 (9)	N2—Zn1—O2	94.60 (10)

All H 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) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXL97*.

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