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Methanol[4-nitro-2-(pyridin-2-ylmethyliminomethyl)phenolato](thiocyanato)zinc(II)

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The title compound, $[Zn(C_{13}H_{10}N_3O_3)(NCS)(CH_4O)]$, is a mononuclear zinc(II) complex. The Zn^{II} atom has a square-pyramidal coordination geometry. In the basal plane, the Zn^{II} atom is coordinated by one O atom and two N atoms of the Schiff base ligand, and by the N atom of a thiocyanate anion. The apical position is occupied by the O atom of a coordinated methanol molecule. In the crystal structure, the molecules are linked *via* intermolecular O—H···O hydrogen bonds, forming chains parallel to the *a* axis.

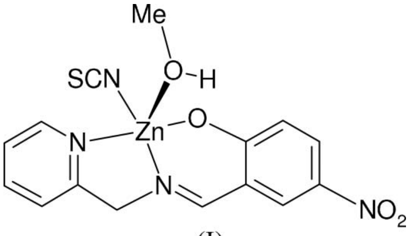
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.108
Data-to-parameter ratio = 16.3

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

Comment

2-(Pyridin-2-ylmethyliminomethyl)phenol (PYMP) is a tridentate Schiff base ligand, which forms stable complexes with a large number of transition metal ions (You, Chen *et al.*, 2004; You & Zhu, 2004). However, complexes related to the PYMP derivative, 4-nitro-2-(pyridin-2-ylmethyliminomethyl)phenol, have seldom been reported. We have focused our attention on the assembly of transition metal ions with flexible Schiff base ligands, since they can adopt diverse coordination modes according to the geometric needs of the metal ions (You, 2005*a*,*b*,*c*). We report a new zinc(II) complex, (I), which is isostructural with the copper(II) complex (Wang & Li, 2005).



(I)

Complex (I) is a mononuclear zinc(II) compound (Fig. 1). The Zn^{II} ion has a square-pyramidal coordination geometry. In the basal plane, the Zn^{II} atom is coordinated by one O atom and two N atoms of the Schiff base ligand, and by the N atom of a thiocyanate anion. The O atom of a coordinated methanol molecule occupies the apical position. A slight distortion of the square pyramid is revealed by the bond angles between the apical and basal donor atoms. The bond angles involving the donor atoms in the basal positions show less distortion. The N2—Zn1—N3 bond angle deviates from 90° by 7.35 (8)°, due to the strain created by the Zn1/N2/C8/C9/N3 five-membered chelate ring. The Zn—O and Zn—N bond lengths (Table 1) are comparable to the corresponding values observed for other Schiff base zinc(II) complexes (Chisholm *et al.*, 2001; Erxleben, 2001; You, Zhu & Liu, 2004). The dihedral angle between the two aromatic rings is 18.9 (1)° and that

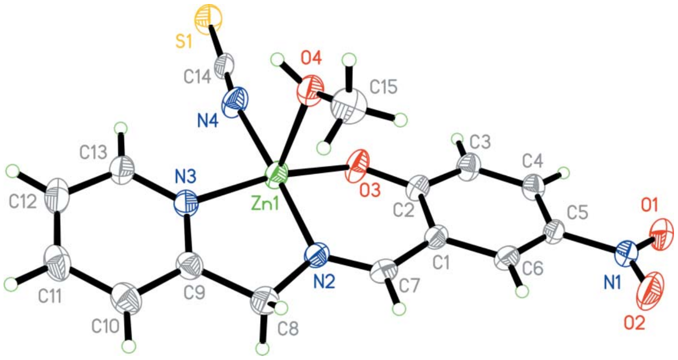


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

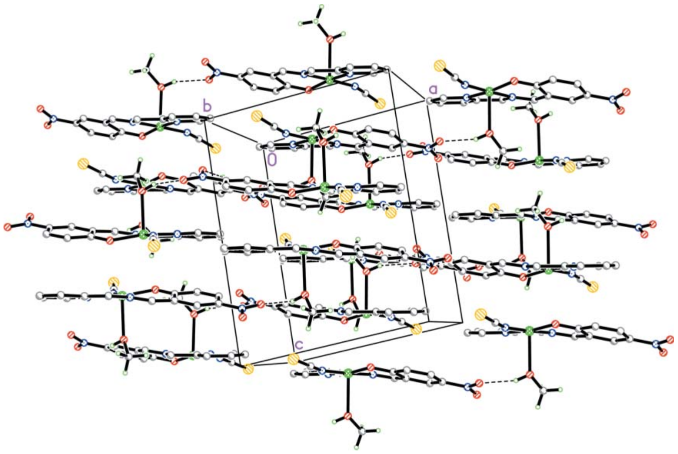


Figure 2
The crystal packing of (I). Intermolecular hydrogen bonds are shown as dashed lines.

between the C1–C6 benzene ring and the O1/N1/O2 plane is 6.8 (2)°.

In the crystal structure of (I), the molecules are linked *via* intermolecular O—H···O hydrogen bonds, forming chains parallel to the *a* axis (Table 2 and Fig. 2).

Experimental

5-Nitrosalicylaldehyde (0.1 mmol, 16.7 mg) and 2-(aminomethyl)pyridine (0.1 mmol, 10.8 mg) were dissolved in methanol (10 ml). The mixture was stirred for 10 min to give a clear yellow solution, which was added to a stirred aqueous solution of NH_4NCS (0.1 mmol, 7.6 mg, 5 ml) and then a solution of $Zn(CH_3COO)_2 \cdot 4H_2O$ (0.1 mmol, 25.6 mg) in methanol (5 ml) was added. The mixture was stirred at room temperature for another 10 min and filtered. The filtrate was kept in air for 3 d, producing colourless block-shaped crystals.

Crystal data

$[Zn(C_{13}H_{10}N_3O_3)(NCS)(CH_4O)]$
M_r = 411.73
Monoclinic, $P2_1/c$
a = 10.617 (1) Å
b = 11.399 (1) Å
c = 13.691 (1) Å
β = 94.133 (1)°
V = 1652.6 (2) Å^3
Z = 4
D_x = 1.655 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5978 reflections
θ = 2.3–28.3°
μ = 1.64 mm^{-1}
T = 298 (2) K
Block, colourless
0.35 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.597, $T_{\max}$ = 0.735
13802 measured reflections
3759 independent reflections
3188 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021
$\theta_{\max}$ = 27.5°
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.05
3759 reflections
230 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.7163P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.46 e Å^{-3}
$\Delta\rho_{\min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3	1.918 (2)	Zn1—N3	2.005 (2)
Zn1—N4	1.941 (2)	Zn1—O4	2.420 (2)
Zn1—N2	1.943 (2)		
O3—Zn1—N4	89.93 (8)	N2—Zn1—N3	82.65 (8)
O3—Zn1—N2	91.59 (7)	O3—Zn1—O4	97.62 (8)
N4—Zn1—N2	177.05 (9)	N4—Zn1—O4	91.61 (9)
O3—Zn1—N3	169.37 (9)	N2—Zn1—O4	90.70 (8)
N4—Zn1—N3	95.45 (9)	N3—Zn1—O4	91.40 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O1$^{\rm i}$	0.84 (1)	2.07 (2)	2.869 (3)	161 (4)

Symmetry code: (i) $x + 1, y, z$.

Atom H4*A* was located in a difference Fourier map and refined isotropically, with $U_{\rm iso}$(H) value fixed at 0.08 Å^2 and the O—H distance restrained to 0.84 (1) Å. The other 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 $U_{\rm iso}$(H) = 1.2 or 1.5$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); 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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