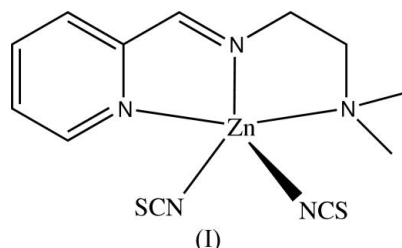


[*N,N'*-Dimethyl-*N''*-(2-pyridylmethylene)-ethane-1,2-diamine]dithiocyanatozinc(II)**Guang Chen,^{a*} Zhi-Ping Bai^b and Sheng-Ju Qu^b**^aDepartment of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China, and ^bCoordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of ChinaCorrespondence e-mail:
qufuchenguang@163.com**Key indicators**Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.039
wR factor = 0.117
Data-to-parameter ratio = 20.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Zn}(\text{NCS})_2(\text{C}_{10}\text{H}_{15}\text{N}_3)]$, is a mononuclear zinc(II) complex. The molecule is isostructural with the analogous copper(II) compound [Yue, Xu, Shi & Feng (2005). *Acta Cryst. E* **61**, m693–m694]. The Zn atom exhibits a square pyramidal geometry.

Comment

Zinc(II) complexes play an important role in numerous biological systems, where they usually function as the active site of hydrolytic enzymes (Casella & Gullotti, 1981; Leussing & Leach, 1971). As a part of our investigations of the structures of zinc derivatives, we have prepared the title compound, (I), a new mononuclear Zn(II) complex (Fig. 1), which is isostructural with the analogous copper(II) complex, [*N,N*-dimethyl-*N''*-(2-pyridylmethylene)ethane-1,2-diamino]dithiocyanatocopper(II), (Yue *et al.*, 2005). All the geometric parameters (Table 1) are within normal ranges (Erxleben, 2001). The Zn atom is five-coordinated by the three N atoms of the Schiff base and the terminal N atoms from two thiocyanate anions, giving a severely distorted square pyramidal geometry.

**Experimental**

N,N'-Dimethylethane-1,2-diamine (0.5 mmol, 44.1 mg) and pyridylaldehyde (0.5 mmol, 53.7 mg) were dissolved in EtOH (35 ml). The mixture was refluxed for 30 min, and aqueous solutions (5 ml) of ammonium thiocyanate (1.0 mmol, 76.2 mg) and $\text{Zn}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (1.0 mmol, 372.4 mg) were added. The mixture was stirred under reflux for another 30 min to give a clear yellow solution. After allowing the solution to stand in air for 15 d, yellow crystals were formed.

Crystal data $[\text{Zn}(\text{NCS})_2(\text{C}_{10}\text{H}_{15}\text{N}_3)]$
M_r = 358.78
Monoclinic, *P*2₁/*n*
a = 10.221 (1) Å
b = 15.054 (2) Å
c = 10.600 (1) Å
 β = 91.190 (1)°
V = 1630.6 (3) Å³
Z = 4*D_x* = 1.461 Mg m⁻³
Mo *K*α radiation
Cell parameters from 5567 reflections
 θ = 2.4–25.1°
 μ = 1.76 mm⁻¹
T = 295 (2) K
Block, yellow
0.22 × 0.13 × 0.11 mm

Data collection

Bruker APEX SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.698$, $T_{\max} = 0.830$
 18260 measured reflections

3732 independent reflections
 2795 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -13 \rightarrow 13$
 $k = -19 \rightarrow 19$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.117$
 $S = 1.03$
 3732 reflections
 183 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.5292P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.07 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—N5	1.962 (3)	Zn1—N1	2.207 (3)
Zn1—N4	1.964 (3)	Zn1—N3	2.224 (3)
Zn1—N2	2.061 (2)		
N5—Zn1—N4	111.14 (14)	N2—Zn1—N1	75.35 (10)
N5—Zn1—N2	135.41 (13)	N5—Zn1—N3	96.65 (11)
N4—Zn1—N2	113.31 (12)	N4—Zn1—N3	101.36 (11)
N5—Zn1—N1	96.39 (11)	N2—Zn1—N3	78.16 (10)
N4—Zn1—N1	96.59 (11)	N1—Zn1—N3	152.25 (9)

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 \AA , and with $U_{\text{iso}}(\text{H})$ set to 1.2 or 1.5 times $U_{\text{eq}}(\text{C})$. The highest electron density peak, $1.07 \text{ e } \text{\AA}^{-3}$, is located 1.14 \AA from atom N1, but no physical significance can be attached to this observation.

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, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

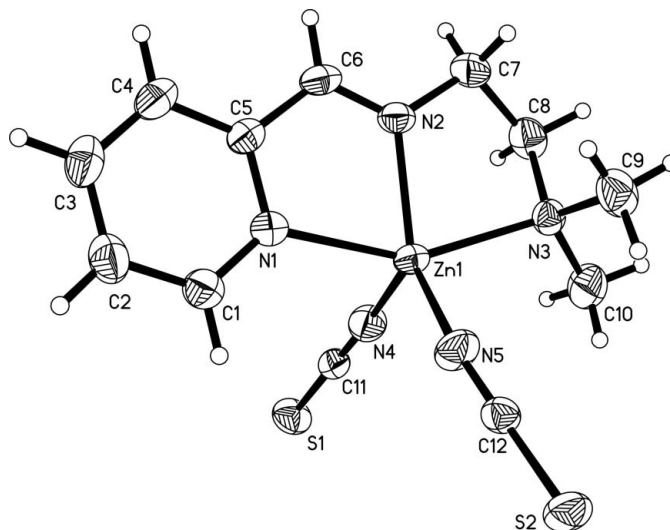


Figure 1

The structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

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References

- Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Casella, L. & Gullotti, M. (1981). *J. Am. Chem. Soc.* **103**, 6338–6347.
- Erxleben, A. (2001). *Inorg. Chem.* **40**, 208–213.
- Leussing, D. L. & Leach, B. E. (1971). *J. Am. Chem. Soc.* **93**, 3377–3384.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). SHELXL97 and SHELXS97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. V5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.
- Yue, G.-R., Xu, X.-J., Shi, Y.-Z. & Feng, L. (2005). *Acta Cryst.* **E61**, m693–m694.