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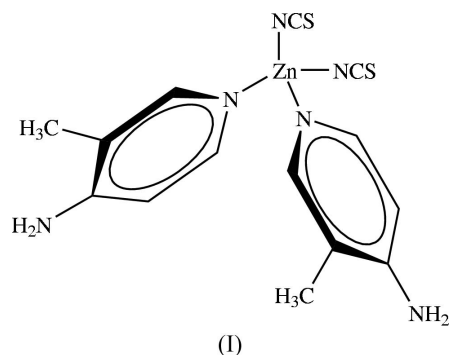
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Key indicatorsSingle-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.031
 wR factor = 0.089
Data-to-parameter ratio = 19.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Bis(4-amino-3-methylpyridine)diisothio-
cyanatozinc(II)**

In the crystal structure of the title compound, $[\text{Zn}(\text{NCS})_2(\text{C}_6\text{H}_8\text{N}_2)_2]$, the Zn atom and both isothiocyanate groups lie on a crystallographic mirror plane. The Zn atom is in a distorted tetrahedral geometry. The crystal structure is stabilized by $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds and weak $\pi-\pi$ interactions.

Comment

A great number of thiocyanate complexes have been synthesized to obtain novel compounds having high stability and special properties (Zhang *et al.*, 1999; Tian *et al.*, 1999). The 4-amino-3-methylpyridine ligand (*L*), which has been synthesized, can emit intense blue-purple fluorescence. $[\text{Zn}(\text{NCS})_2L_2]$, (I), has been synthesized and characterized by X-ray analysis, since it is expected to be a novel complex with high non-linear optical behavior, thermal stability and exhibiting fluorescence. In this paper, the synthesis and crystal structure of (I) is reported.



The Zn atom and both isothiocyanate groups lie on a crystallographic mirror plane at $y = \frac{1}{4}$. The bond lengths and angles of (I) (Table 1) have normal values (Allen *et al.*, 1987). The environment around the Zn atom is that of a distorted tetrahedron, comparable to a related structure of a cadmium thiocyanate polymer (Zhang *et al.*, 1999). The four ligands coordinate to the Zn atom through N atoms, the four N—Zn—N bond angles ranging from 106.77 (6) to 115.78 (9)° (Table 1).

In the crystal structure, the molecules are linked together through intermolecular $\text{N4}-\text{H2B}\cdots\text{S2}$ interactions (Table 2). Weak $\pi-\pi$ interactions exist between parallel pyridine rings, the shortest distance between such rings being 4.493 (1) Å.

Experimental

L (0.4 g) and zinc thiocyanate (0.09 g, molar ratio 2:1) were added to dry methanol (50 ml). The mixture was refluxed and stirred for 4 h.

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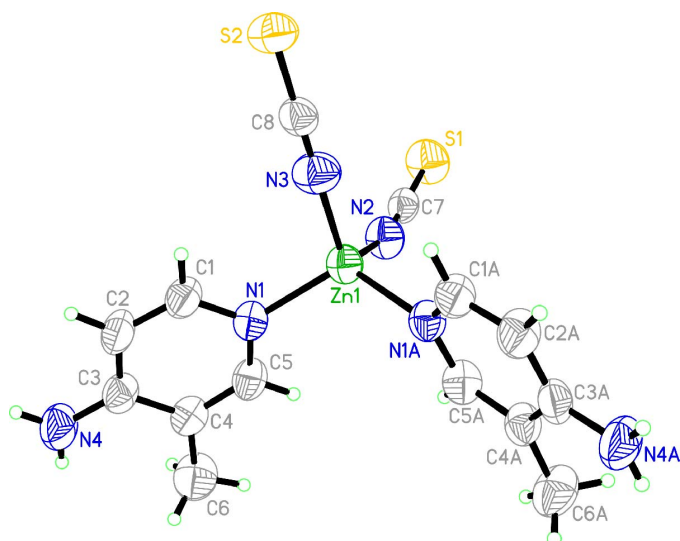


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix A indicates the symmetry code ($x, \frac{1}{2} - y, z$).

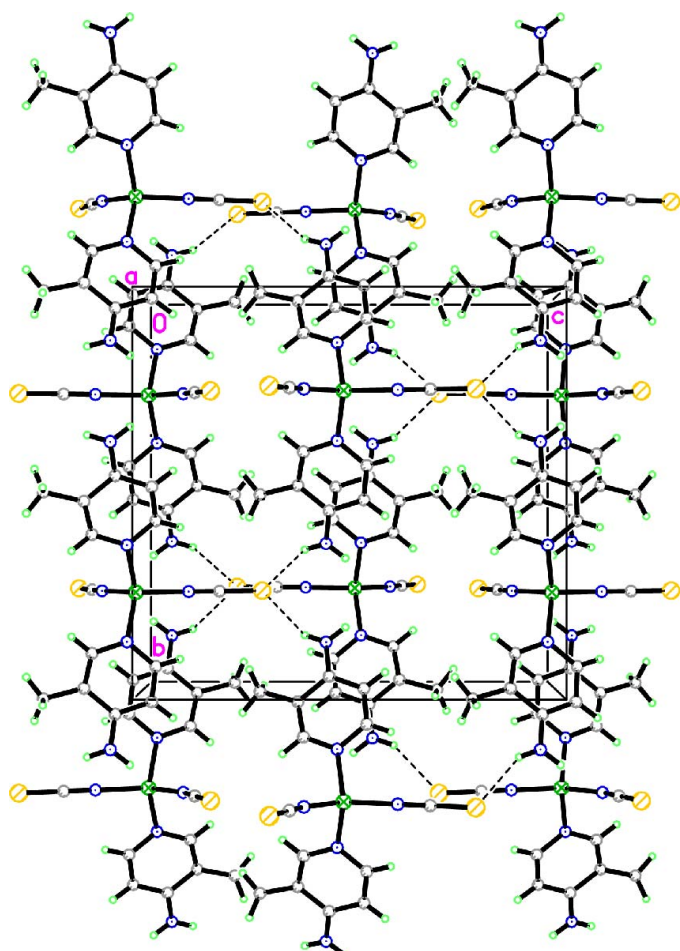


Figure 2
The packing of (I), viewed down the a axis. Hydrogen bonds are shown as dashed lines.

On cooling to room temperature, it yielded pale yellow crystals. Single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of a propanone solution of the complex.

Crystal data

[Zn(NCS)₂(C₆H₈N₂)₂]
 $M_r = 397.82$
 Orthorhombic, $Pnma$
 $a = 8.5622$ (4) Å
 $b = 14.0393$ (7) Å
 $c = 14.7524$ (7) Å
 $V = 1773.35$ (15) Å³
 $Z = 4$
 $D_x = 1.490$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 2289 reflections
 $\theta = 2.8$ – 28.3°
 $\mu = 1.63$ mm⁻¹
 $T = 293$ (2) K
 Block, pale yellow
 $0.48 \times 0.46 \times 0.42$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.463$, $T_{\max} = 0.505$
 10596 measured reflections

2289 independent reflections
 1934 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 28.3^\circ$
 $h = -10 \rightarrow 11$
 $k = -11 \rightarrow 18$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.089$
 $S = 1.07$
 2289 reflections
 116 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.5026P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.65$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1–N3	1.958 (3)	N1–C1	1.340 (2)
Zn1–N2	1.963 (3)	N1–C5	1.347 (2)
Zn1–N1	2.0028 (16)	N2–C7	1.147 (4)
S1–C7	1.607 (3)	N3–C8	1.152 (4)
S2–C8	1.616 (3)	N4–C3	1.347 (3)
N3–Zn1–N2	112.11 (11)	N1–Zn1–N1 ⁱ	115.78 (9)
N3–Zn1–N1	106.77 (6)	C7–N2–Zn1	161.1 (2)
N2–Zn1–N1	107.76 (6)	C8–N3–Zn1	179.3 (3)

Symmetry codes: (i) $x, \frac{1}{2} - y, z$.

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N4–H4B ⁱⁱ ··S2 ⁱⁱ	0.86	2.81	3.591 (2)	152

Symmetry code: (ii) $\frac{1}{2} - x, -y, \frac{1}{2} + z$.

H atoms were positioned geometrically and were treated as riding on their parent atoms, with C–H = 0.93 (aromatic) and 0.96 Å (methyl), and N–H = 0.86 Å, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl H atoms and $1.2U_{\text{eq}}(\text{C}, \text{N})$ for other H atoms. A rotating group model was used for the methyl groups.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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