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Bis(3-aminopyridine-κ*N*)diisothiocyanatozinc(II)

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In the title compound, $[Zn(NCS)_2(C_5H_6N_2)_2]$, the Zn atom adopts a distorted tetrahedral coordination geometry and is bonded to two N atoms from thiocyanate anions and two pyridyl N atoms. The Zn atom and the two thiocyanate ligands are located on a mirror plane. The crystal structure is stabilized by N—H···S hydrogen bonds.

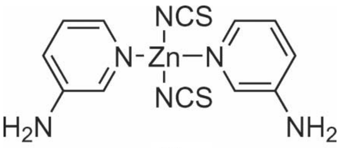
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.087
Data-to-parameter ratio = 13.9

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

Comment

The crystal engineering of supramolecular architectures based on metals and organic building blocks has rapidly developed in recent years owing to their novel diverse topologies and potential applications in fields such as catalysis, molecular recognition and molecular separations (Fujita *et al.*, 1994; Evans & Lin, 2002). A variety of topologies of metal–organic complexes are highly influenced by many factors such as the structures of the organic ligands, the coordination geometries of the metal ions, the solvent system and the counter-anions. 3-Aminopyridine and thiocyanate as bidentate ligands have been used as versatile organic blocks because these ligands show different coordination modes and generate many new supramolecular structures under different conditions (Horikoshi & Mikuriya, 2005). We report here the crystal structure of a zinc(II) complex with these two ligands, (I).



(I)

The Zn atom adopts a distorted tetrahedral coordination geometry and is bonded to two N atoms from the thiocyanate anions and two pyridyl N atoms (Fig. 1). The Zn atom and the two thiocyanate ligands are located on a mirror plane. The Zn—N1(pyridyl) bond length is 2.018 (2) Å and the Zn—NCS bond lengths are almost equal, at 1.952 (4) Å for N3 and 1.932 (3) Å for N4, respectively. The N—Zn—N angles are in the range 103.33 (8)–118.92 (15)°. The dihedral angles between the plane containing Zn1 and thiocyanate ligands and the pyridine plane is 56.02 (5)°. All bond distances and angles are as observed for the other zinc(II) complexes with pyridine and thiocyanate ligands (Chantrapromma *et al.*, 2005; Fettouhi, 2000; Fettouhi *et al.*, 2002; Hou *et al.*, 2003; Secondo *et al.*, 2000; Wu, 2004). The crystal structure is stabilized by N—H···S hydrogen bonds (Table 1 and Fig. 2).

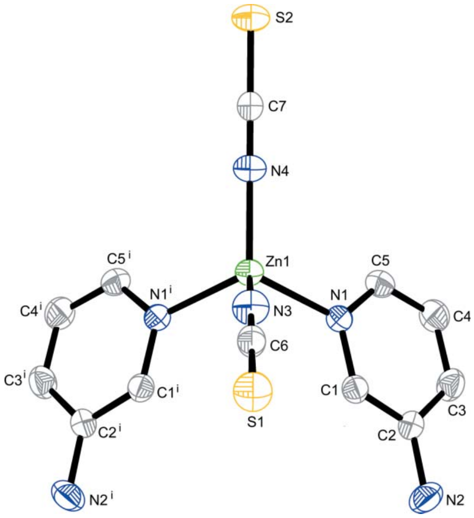


Figure 1
The molecular structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $x, \frac{3}{2} - y, z$.]

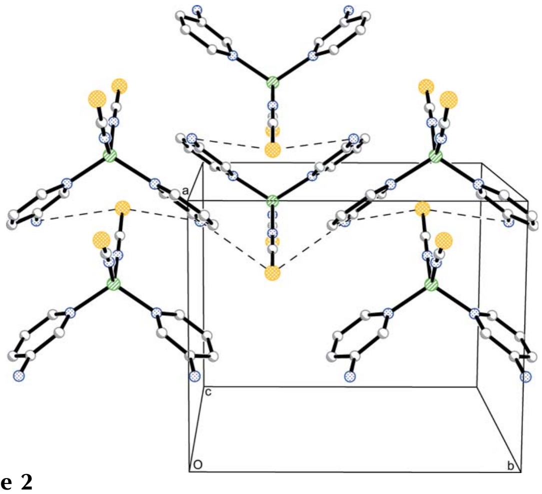


Figure 2
A packing diagram for (I). Dashed lines indicate hydrogen bonds. H atoms have been omitted for clarity.

Experimental

A mixture of $ZnCl_2\cdot6H_2O$ (0.488 g, 2 mmol), 3-aminopyridine (2 mmol, 0.188 g), NH_4SCN (10 mmol, 0.152 g) and methanol (10 ml) was stirred for 1 h at room temperature. The reaction was carried out in a Teflon-lined steel autoclave, which was heated at 450 K for 2 d followed by slow cooling to room temperature. The resulting colorless block-shaped crystals suitable for X-ray analysis were filtered off and washed with water (yield 68.5% based on Zn). Analysis, calculated for $C_{12}H_{12}N_6S_2Zn$: C 38.98, H 3.27, N 22.73%; found: C 38.85, H 3.39, N 22.68%.

Crystal data

$[Zn(NCS)_2(C_5H_6N_2)_2]$
$M_r = 369.77$
Orthorhombic, *Pnma*
$a = 10.174$ (3) Å
$b = 12.312$ (3) Å
$c = 12.711$ (4) Å
$V = 1592.2$ (8) Å^3
$Z = 4$
$D_x = 1.543$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.81$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.46 × 0.43 × 0.39 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.491$, $T_{max} = 0.539$ (expected range = 0.450–0.494)
7856 measured reflections
1469 independent reflections
1107 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.087$
$S = 1.09$
1469 reflections
106 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.5218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···S1^{i}	0.86	2.73	3.578 (3)	170
N2—H2*A*···S2^{ii}	0.86	3.01	3.777 (3)	150

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $x - \frac{1}{2}, y, -z + \frac{3}{2}$.

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = $1.2U_{eq}$(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: *SHELXTL*.

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