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Tetrapyridinedithiocyanatozinc(II)

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Key indicators

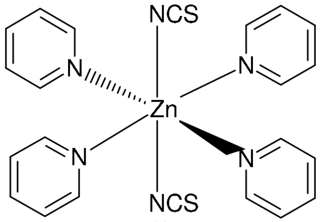
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.061
wR factor = 0.181
Data-to-parameter ratio = 15.9

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

The title compound, $[Zn(NCS)_2(C_5H_5N)_4]$, is a mononuclear zinc complex. The Zn^{II} atom, lying on an inversion centre, is six-coordinated by four N atoms from four pyridine ligands and by another two N atoms from two thiocyanate anions in a slightly distorted octahedral geometry.

Comment

Transition metal complexes are very important in the development of the coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Zinc, the second most abundant transition metal in biology, functions as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase, where it is in a hard-donor coordination environment of N and O (Lipscomb & Sträter, 1996). Zinc has long been recognized as an important cofactor in biological molecules, either as a structural template in protein folding or as a Lewis acid catalyst that can readily adopt four-, five- or six-coordination (Vallee & Auld, 1993). Recent reports have suggested that zinc is able to play a catalytic role in the activation of thiols as nucleophiles at physiological pH (Matthews & Goulding, 1997; Wilker & Lippard, 1997; Myers *et al.*, 1993). As an extension of the work on the structural characterization of zinc(II) complexes, the synthesis and structure of the title compound, (I), are reported here.



(I)

The title compound is a centrosymmetric zinc complex (Fig. 1). The Zn^{II} atom, with site symmetry $\overline{1}$, is octahedrally coordinated by four N atoms from four pyridine ligands and by another two N atoms from two monodentate thiocyanate anions. The *cis*-octahedral bond angles around Zn are close to 90°, varying from 87.18 (12) to 92.82 (12)°, which indicates a slightly distorted octahedral geometry. The Zn1—N1(pyridine) bond length in (I) is slightly shorter than the value of 2.243 (3) Å observed in a related zinc complex (Ali *et al.*, 2004). The Zn1—N3(thiocyanate) bond length is also a little shorter than the value of 2.103 (7) Å observed in another related zinc(II) complex (Lu *et al.*, 1998). The unit-cell packing of (I) is shown in Fig. 2.

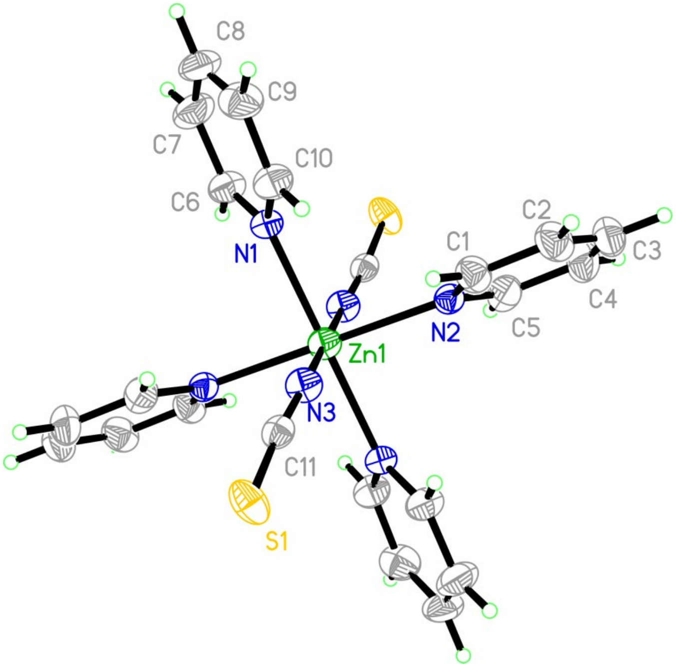


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids (small spheres for the H atoms) and the atom-numbering scheme. Only one component of the disordered S atom is shown.

Experimental

Pyridine (0.2 mmol, 15.8 mg) and ammonium thiocyanate (0.1 mmol, 6.0 mg) were dissolved in methanol and a methanol solution of $Zn(CH_3COO)_2 \cdot 2H_2O$ (0.1 mmol, 22.0 mg) was added with stirring. The resulting mixture was stirred for 1 h at room temperature to give a clear yellow solution. The solution was kept in air for 15 d, during which time yellow block-shaped crystals of (I) were formed on slow evaporation of the solvent.

Crystal data

$[Zn(NCS)_2(C_5H_5N)_4]$
$M_r = 497.93$
Monoclinic, $C2/c$
$a = 12.396\ (7)$ Å
$b = 13.022\ (7)$ Å
$c = 15.148\ (8)$ Å
$\beta = 107.478\ (10)^\circ$
$V = 2332\ (2)$ Å^3
$Z = 4$

$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1794 reflections
$\theta = 2.3$–22.8°
$\mu = 1.25$ mm^{-1}
$T = 273\ (2)$ K
Block, yellow
0.22 × 0.14 × 0.12 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.770$, $T_{\max} = 0.864$
6602 measured reflections

2397 independent reflections
1817 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 26.5^\circ$
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 15$
$l = -12 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.181$
$S = 1.09$
2397 reflections
151 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0977P)^2 + 2.3125P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.41$ e Å^{-3}

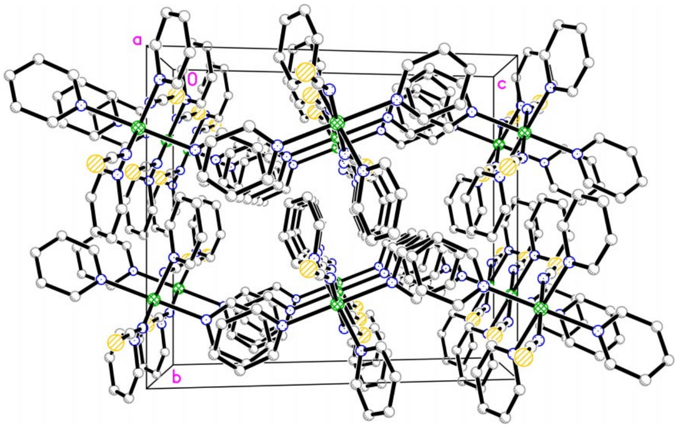


Figure 2
The unit cell contents of (I), viewed along the *a* axis, with H atoms omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	2.071 (3)	Zn1—N2	2.211 (3)
Zn1—N1	2.204 (3)		
N3—Zn1—N1$^{\rm i}$	89.32 (14)	N3$^{\rm i}$—Zn1—N2	89.25 (13)
N3—Zn1—N1	90.68 (14)	N1$^{\rm i}$—Zn1—N2	87.18 (12)
N3—Zn1—N2	90.75 (13)	N1—Zn1—N2	92.82 (12)

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$. The occupancies of the disordered S1/S1′ atoms of the thiocyanate moiety were both fixed at 0.5.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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