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[4′-(4-Pyridyl)-2,2′:6′,2″-terpyridine-κ^3N,N',N'']-dithiocyanatozinc(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 13.2

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

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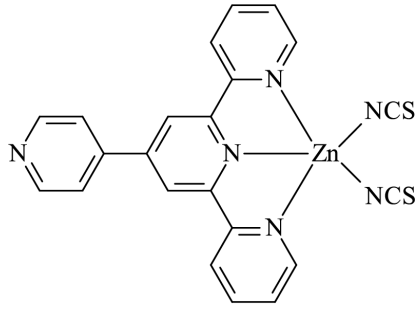
In the title complex, $[Zn(NCS)_2(C_{20}H_{14}N_4)]$, the Zn^{II} atom is coordinated by a tridentate chelating 4′-(4-pyridyl)-2,2′:6′,2″-terpyridine (pyterpy) ligand and two thiocyanate groups, to form a distorted trigonal–bipyramidal coordination geometry.

Comment

The ligand 4′-(4-pyridyl)-2,2′:6′,2″-terpyridine (pyterpy) contains two discrete metal-binding domains, as expected, which would result in macrocyclic oligomers or linear polymers through coordination of the monodentate pendant pyridyl group (Sun & Lees, 2001; Hayami *et al.*, 2004). As a continuing effort of our research on complexes of terpyridine derivatives (Hou, Li, Wu *et al.*, 2004; Hou, Li, Yin *et al.*, 2004; Tu *et al.*, 2004), we report here the mononuclear complex [4′-(4-pyridyl)-2,2′:6′,2″-terpyridine-κ^3N,N',N'']dithiocyanatozinc(II), (I), using this ligand.



(I)

In complex (I), the Zn center is coordinated by three N atoms from the pyterpy ligand and two N atoms from two thiocyanate groups, displaying a distorted trigonal–bipyramidal geometry. The two axial sites are occupied by the terminal pyridyl N atoms of the pyterpy ligand, with Zn—N distances [2.159 (2) and 2.182 (3) Å] which are longer than the equatorial Zn—N distance [2.089 (2) Å] to the central pyridyl ring, as a consequence of the rigid structure of the terpyridyl unit. The values of the bite angles of the terpyridyl unit are 74.8 (1) and 74.9 (1)°.

Experimental

The 4′-(4-pyridyl)-2,2′:6′,2″-terpyridine ligand was synthesized according to a literature method (Constable & Thompson, 1992). A mixture of zinc chloride (0.027 g, 0.2 mmol), pyterpy (0.062 g, 0.2 mmol), ammonium thiocyanate (0.017 g, 0.4 mmol) and water (10 ml) was heated to 413 K for 72 h, and then cooled to room temperature at a rate of 1 K every 10 min. X-ray quality yellow crystals of the compound were obtained in *ca* 75% yield.

Crystal data

$[Zn(NCS)_2(C_{20}H_{14}N_4)]$	$Z = 2$
$M_r = 491.88$	$D_x = 1.543$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.5358$ (7) Å	Cell parameters from 2515 reflections
$b = 10.7110$ (8) Å	$\theta = 2.2$–$23.3°$
$c = 12.2233$ (9) Å	$\mu = 1.38$ mm^{-1}
$\alpha = 65.862$ (1)°	$T = 295$ (2) K
$\beta = 68.360$ (1)°	Block, yellow
$\gamma = 80.330$ (1)°	0.24 × 0.18 × 0.15 mm
$V = 1058.8$ (1) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	3704 independent reflections
	3131 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$\theta_{max} = 25.0°$
	$h = -11 \rightarrow 11$
$T_{min} = 0.702$, $T_{max} = 0.820$	$k = -12 \rightarrow 12$
7692 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
3704 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
280 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.159 (2)	Zn1—N5	1.979 (3)
Zn1—N2	2.089 (2)	Zn1—N6	1.965 (3)
Zn1—N3	2.181 (3)		
N1—Zn1—N2	74.9 (1)	N2—Zn1—N5	119.2 (1)
N1—Zn1—N3	149.5 (1)	N2—Zn1—N6	130.5 (1)
N1—Zn1—N5	99.6 (1)	N3—Zn1—N5	97.2 (1)
N1—Zn1—N6	98.8 (1)	N3—Zn1—N6	99.0 (1)
N2—Zn1—N3	74.8 (1)	N5—Zn1—N6	110.3 (1)

H atoms were placed at calculated positions [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$] and were refined using the riding-model approximation.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

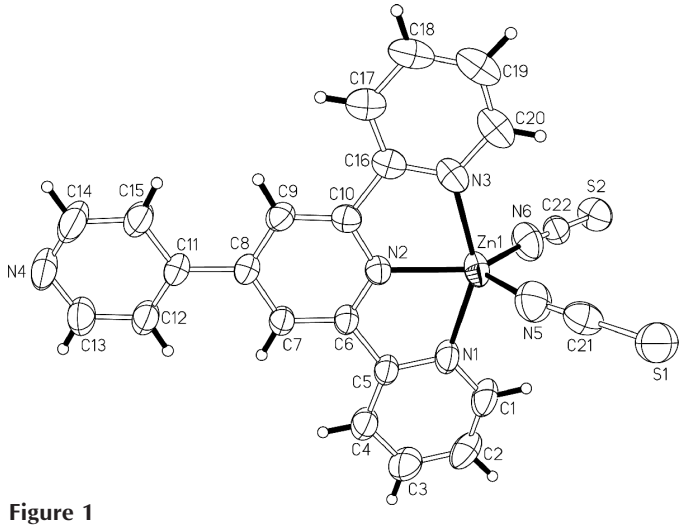


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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