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

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.134
Data-to-parameter ratio = 16.7

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

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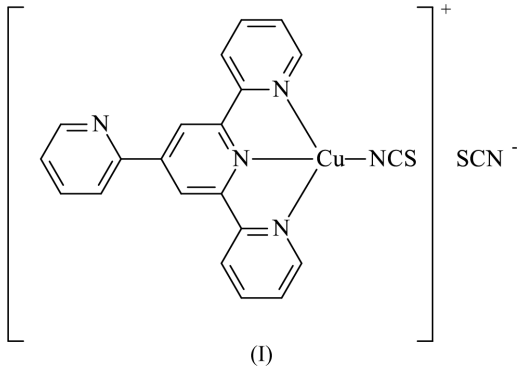
In the title compound, [Cu(NCS)($C_{20}H_{14}N_4$)]SCN, the Cu atom is four-coordinated by a tridentate chelating 4′-(2-pyridyl)-2,2′:6′,2″-terpyridine ligand and one isothiocyanate group in a square-planar coordination geometry. The sum of angles around the Cu^{II} center is 359.1°.

Comment

2,2′:6′,2″-Terpyridine has a rigid, easily substituted structure that makes it an attractive target for use in the synthesis of functional materials (Andres & Schubert, 2004). We have previously studied terpyridine derivatives as tridentate chelating units coordinated to Zn^{II}, Cu^{II} and Ag^{I} (Hou, Li & Ng, 2004; Hou, Li, Wu *et al.*, 2004; Hou, Li, Yin *et al.*, 2004). In this work, we report a new complex, (I), incorporating the 4′-(2-pyridyl)-2,2′:6′,2″-terpyridine ligand.



(I)

In complex (I), the Cu^{II} center is coordinated by three N atoms from the terpyridine ligand and one N atom from an isothiocyanate group, displaying a square-planar geometry (Fig. 1). The Cu—N bond lengths defined by the ligand are in the range 1.924 (3)–2.029 (3) Å; the shortest distance is between copper and the central pyridine and is characteristic of terpyridine complexes. The values of the angles subtended by the terpyridine unit [79.8 (1) and 80.0 (1)°] deviate from the ideal value of 90° mainly as a consequence of the geometric constraints imposed by the ligand. The free thiocyanate counter-ion is involved in a Cu···S contact, with a Cu···S separation of 2.819 (1) Å.

Experimental

4′-(2-Pyridyl)-2,2′:6′,2″-terpyridine was synthesized according to a modified literature method (Constable & Thompson, 1992). The ligand (0.031 g, 0.1 mmol) was dissolved in 5 ml tetrahydrofuran and layered on to a saturated potassium thiocyanate solution (5 ml) containing cuprous thiocyanate (0.012 g, 0.1 mmol). The solution was

left for two weeks at room temperature and green crystals were obtained in about 60% yield.

Crystal data

$[Cu(NCS)(C_{20}H_{14}N_4)]SCN$	$D_x = 1.581$ Mg m^{-3}
$M_r = 490.05$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2798 reflections
$a = 8.6898$ (6) Å	$\theta = 2.7$–$27.2°$
$b = 30.008$ (2) Å	$\mu = 1.29$ mm^{-1}
$c = 8.1262$ (6) Å	$T = 295$ (2) K
$\beta = 103.622$ (1)°	Block, green
$V = 2059.4$ (3) Å^3	0.20 × 0.18 × 0.15 mm
$Z = 4$	

Data collection

Bruker SMART APEX area-detector diffractometer	4685 independent reflections
	3677 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.029$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$\theta_{max} = 27.5°$
	$h = -9 \rightarrow 11$
$T_{min} = 0.240$, $T_{max} = 0.830$	$k = -32 \rightarrow 38$
12864 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 1.0711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	
$wR(F^2) = 0.134$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.75$ e Å^{-3}
4685 reflections	$\Delta\rho_{min} = -0.58$ e Å^{-3}
280 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.029 (3)	Cu1—N3	2.029 (3)
Cu1—N2	1.924 (2)	Cu1—N5	1.909 (3)
N1—Cu1—N2	80.0 (1)	N2—Cu1—N3	79.8 (1)
N1—Cu1—N3	158.9 (1)	N2—Cu1—N5	173.0 (1)
N1—Cu1—N5	99.7 (1)	N3—Cu1—N5	99.6 (1)

H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}$(C)], and were included in the refinement in 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.

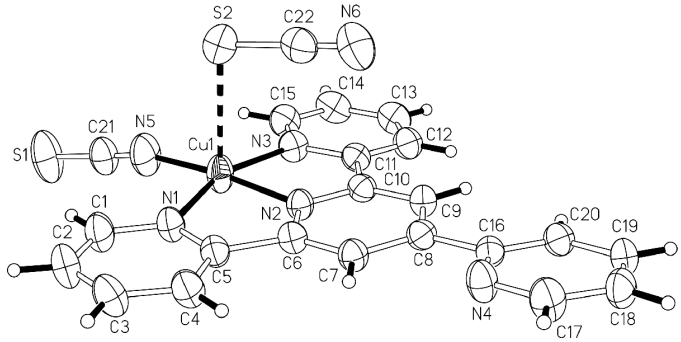


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. The dashed line indicates the short Cu···S contact.

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References

Andres, P. R. & Schubert, U. S. (2004). *Adv. Mater.* **16**, 1043–1068.
Bruker (2002). *SADABS, SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Constable, E. C. & Thompson, A. M. W. C. (1992). *J. Chem. Soc. Dalton Trans.* pp. 2947–2950.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Hou, L., Li, D. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m1734–m1735.
Hou, L., Li, D., Wu, T., Yin, Y.-G. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m1181–m1182.
Hou, L., Li, D., Yin, Y.-G., Wu, T. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m1106–m1107.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.