

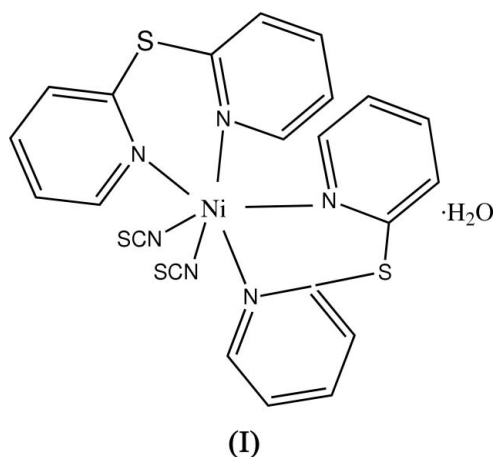
Qi-Hua Zhao,* Xiu-Mei Mu,
Mei-Su Zhang and Rui-Bing FangDepartment of Chemistry, Centre for Advanced
Studies of Medicinal and Organic Chemistry,
Yunnan University, Kunming 650091, People's
Republic of China

Correspondence e-mail: qhzhao@ynu.edu.cn

Key indicators

Single-crystal X-ray study
 $T = 289\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
H-atom completeness 89%
Disorder in solvent or counterion
 R factor = 0.039
 wR factor = 0.105
Data-to-parameter ratio = 18.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(thiocyanato- κN)bis(2,2'-thiodipyridine- $\kappa^2\text{N},\text{N}'$)-
nickel(II) monohydrateIn the title complex, $[\text{Ni}(\text{NCS})_2(\text{C}_{10}\text{H}_8\text{N}_2\text{S})_2]\cdot\text{H}_2\text{O}$, the Ni^{II} ion is coordinated by four pyridine N and two thiocyanate N atoms in a distorted octahedral geometry. The Ni—N(pyridine) bond lengths are significantly longer than the Ni—N(NCS) bond lengths.Received 11 November 2005
Accepted 21 February 2006

Comment

Recently, several metal complexes incorporating thio-dipyridine (tbp) have been reported (Jung *et al.*, 2001, 2003). We present here the crystal structure of the title complex, (I), incorporating the 2,2'-tbp ligand.

The molecular structure of (I) is shown in Fig. 1. While two tbp ligands chelate to the Ni^{II} ion through the pyridine N atoms, two thiocyanate N atoms *cis*-coordinate to the Ni^{II} ion to complete the distorted octahedral coordination geometry (Table 1). The Ni—N(pyridine) bond lengths are significantly longer than the Ni—N(NCS) bond lengths. Within each tbp ligand, the two pyridine rings are tilted with respect to one another, with dihedral angles of $44.26(8)$ and $53.15(11)^\circ$ for S1-tbp and S2-tbp, respectively.

Experimental

An acetone solution (5 ml) of thiodipyridine (0.4 mmol, 75.3 mg) was mixed with an ethanol solution (10 ml) of $\text{Ni}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.2 mmol, 58.2 mg). The mixture was stirred for 1 h at room temperature. An ethanol solution (5 ml) of KSCN (0.4 mmol, 38.9 mg) was then added dropwise to the mixture and it was stirred for a further 1.5 h. Blue single crystals of (I) were obtained by slow evaporation of the solution at room temperature (yield 40.3%).

Crystal data

[Ni(NCS)₂(C₁₀H₈N₂S)₂]·H₂O
M_r = 569.38
 Monoclinic, *P*2₁/*c*
a = 8.3379 (5) Å
b = 29.3927 (19) Å
c = 10.2119 (7) Å
 β = 95.147 (1)°
V = 2492.6 (3) Å³
Z = 4

D_x = 1.517 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 4506 reflections
 θ = 2.4–25.4°
 μ = 1.14 mm⁻¹
T = 289 (2) K
 Block, blue
 0.38 × 0.26 × 0.14 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.705, *T_{max}* = 0.850
 16243 measured reflections

5708 independent reflections
 4345 reflections with *I* > 2σ(*I*)
R_{int} = 0.023
 θ_{max} = 27.5°
h = -10 → 10
k = -38 → 36
l = -13 → 9

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.039
wR(*F*²) = 0.105
S = 1.04
 5708 reflections
 317 parameters
 H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0512*P*)² + 1.153*P*]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δσ)_{max} = 0.002
 Δρ_{max} = 0.50 e Å⁻³
 Δρ_{min} = -0.60 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1–N1	2.129 (2)	Ni1–N4	2.126 (2)
Ni1–N2	2.129 (2)	Ni1–N5	2.050 (2)
Ni1–N3	2.103 (2)	Ni1–N6	2.065 (2)
N5–Ni1–N6	91.57 (10)	N4–Ni1–N1	178.10 (8)
N5–Ni1–N3	176.72 (9)	N5–Ni1–N2	88.62 (9)
N6–Ni1–N3	87.04 (8)	N6–Ni1–N2	177.23 (9)
N5–Ni1–N4	90.24 (9)	N3–Ni1–N2	92.91 (8)
N6–Ni1–N4	89.89 (8)	N4–Ni1–N2	92.87 (8)
N3–Ni1–N4	86.79 (8)	N1–Ni1–N2	85.29 (8)
N5–Ni1–N1	89.29 (9)	C6–S1–C5	103.31 (12)
N6–Ni1–N1	91.95 (8)	C16–S2–C15	105.62 (11)
N3–Ni1–N1	93.73 (8)		

The water molecule is disordered over two sites; the occupancies were refined and converged to 0.54 (2) and 0.46 (2). The H atoms attached to the disordered O atoms were not located. Aromatic H atoms were placed in calculated positions, with C–H = 0.93 Å, and refined in riding mode, with *U*_{iso}(H) = 1.2*U*_{eq}(C).

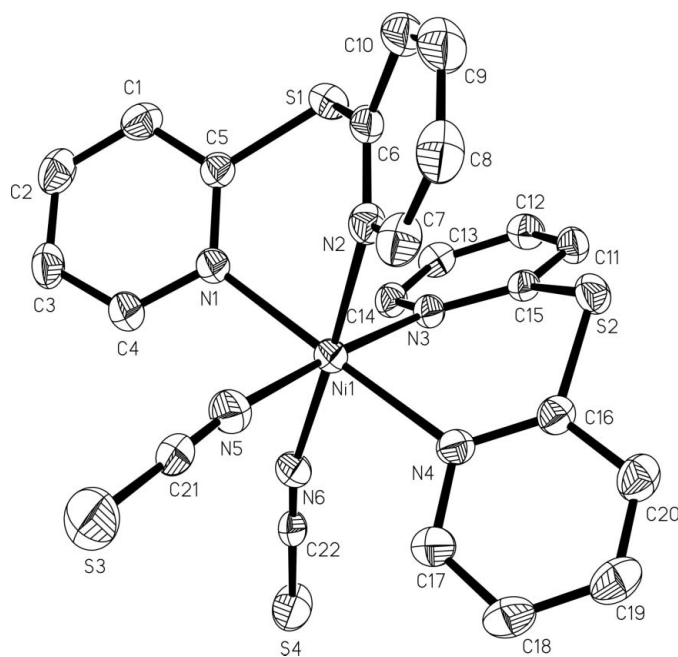


Figure 1
 The molecular structure of (I), with 30% probability displacement ellipsoids. H atoms and the water molecule have been omitted for clarity.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

This work is supported by the NNSFC (Nos. 20361004 and 20561004) and NSF of Yunnan Province (Nos. 2003E0012M, 2004E0008M and 2003RC13).

References

Bruker (1998). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
 Jung, O. S., Kim, Y. J., Lee, Y. A., Chae, H. K., Jang, H. G. & Hong, J. K. (2001). *Inorg. Chem.* **40**, 2105–2110.
 Jung, O. S., Kim, Y. J., Lee, Y. A., Park, K. M. & Lee, S. S. (2003). *Inorg. Chem.* **42**, 844–850.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.