

Fa-Qian Liu,^a Fang-Fang Jian,^b
Guang-Ye Liu,^b Lu-De Lu,^{a*}
Xu-Jie Yang^a and Xin Wang^a

^aMaterials Chemistry Laboratory, Nanjing University of Science and Technology, Nanjing 210094, People's Republic of China, and ^bNew Materials and Functions, Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: fqliu@vip.163.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.008$ Å
 R factor = 0.052
 wR factor = 0.162
Data-to-parameter ratio = 18.2

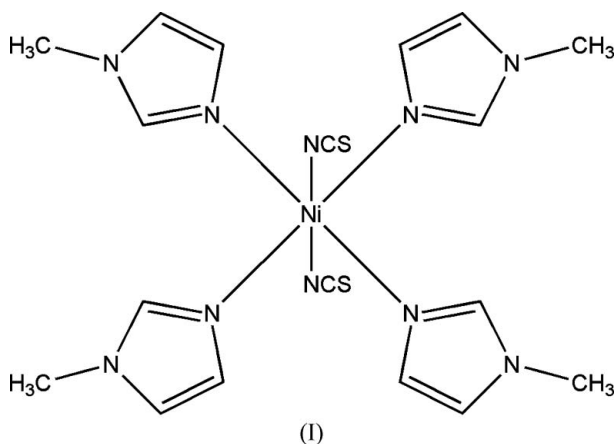
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Diisothiocyanatotetrakis(1-methyl-1*H*-imidazole- κ N³)nickel(II)

The structure of the title compound, $[\text{Ni}(\text{NCS})_2(\text{C}_4\text{H}_6\text{N}_2)_4]$, consists of isolated molecules of $[\text{Ni}(\text{NCS})_2(\text{Mim})_4]$ (Mim = 1-methylimidazole), which contain a compressed octahedral NiN_6 chromophore. The NCS^- anions are *trans* and four N atoms from the 1-methylimidazole ligands define the equatorial plane. The mean $\text{Ni}-\text{N}(\text{Mim})$ and $\text{Ni}-\text{N}(\text{NCS})$ distances are 2.115 (4) and 2.087 (4) Å, respectively.

Comment

Imidazole is of considerable interest as a ligand in many biological systems in which it provides a potential binding site for metal ions (Brooks & Davidson, 1960). Imidazole itself is a unidentate ligand and forms complexes with metal ions through its tertiary N atoms. It has been reported that a large number of imidazole derivatives possesses diverse pharmacological effects, including anti-inflammatory, antimalarial and antitumour activities (Eilbeck *et al.*, 1967; Davis & Smith, 1971). Furthermore, the isothiocyanate anion is a versatile inorganic ligand in the synthesis of coordination compounds. It therefore appeared to be interesting to study the conditions of the formation of thiocyanate-containing nickel(II) complexes with imidazole derivatives, and to investigate the influence of steric properties on the stoichiometry as well as on the structure of the resulting species (Maslejova *et al.*, 1997). Recently, we have reported the crystal structure of the complex $[\text{Co}(\text{NCS})_2(2\text{-methylimidazole})_2]$ (Liu *et al.*, 2005). In this paper, we report the crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The Ni atom displays a compressed octahedral coordination geometry, with six N atoms from two thiocyanate anions and four 1-methylimidazole ligands building the NiN_6 chromo-

Received 24 June 2005

Accepted 8 July 2005

Online 16 July 2005

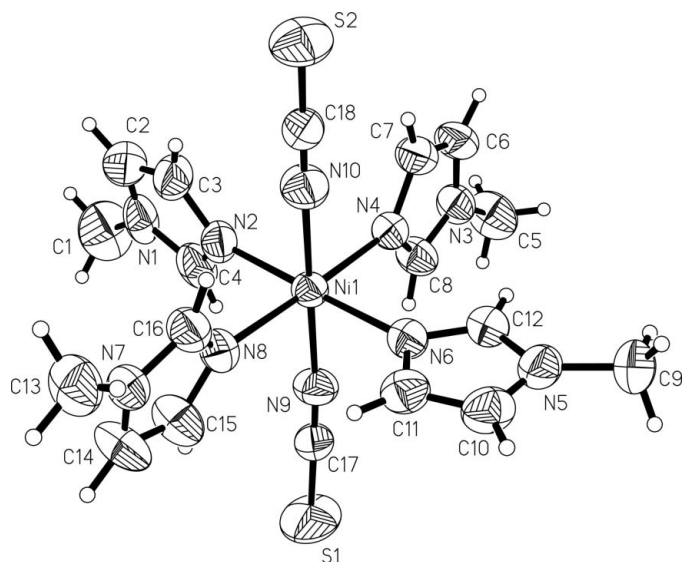


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

phore. The equatorial plane of the complex is formed by four Ni–N(1-methylimidazole) bonds with lengths ranging from 2.103 (4) to 2.129 (4) Å, and the axial positions are occupied by two N-bonded NCS groups [Ni–N(NCS) = 2.083 (4) and 2.091 (4) Å]. These values agree well with those observed in tetrakis(imidazole)bis(isothiocyanato)nickel(II) (Koman *et al.*, 1991). The values of the bond angles around nickel are close to those expected for a regular octahedral geometry (Table 1), the largest angular deviation being observed for the N4–Ni–N8 angle [177.80 (15)°]. The thiocyanate ligands are almost linear (Table 1).

Experimental

The title compound was prepared by the reaction of 1-methylimidazole (1.64 g, 20 mmol) with NiCl₂·6H₂O (1.19 g, 5 mmol) and potassium thiocyanate (0.98 g, 10 mmol) by means of hydrothermal synthesis in a stainless steel reactor with a Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

Crystal data

[Ni(NCS) ₂ (C ₄ H ₆ N ₂) ₄]	$D_x = 1.392 \text{ Mg m}^{-3}$
$M_r = 503.30$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
$a = 11.002 (2) \text{ \AA}$	$\theta = 4\text{--}14^\circ$
$b = 15.300 (3) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$c = 14.309 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 94.28 (3)^\circ$	Block, blue
$V = 2401.9 (8) \text{ \AA}^3$	$0.35 \times 0.25 \times 0.25 \text{ mm}$
$Z = 4$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{\text{max}} = 27.0^\circ$
ω scans	$h = 0 \rightarrow 14$
Absorption correction: none	$k = 0 \rightarrow 19$
5451 measured reflections	$l = -17 \rightarrow 18$
5188 independent reflections	3 standard reflections
2901 reflections with $I > 2\sigma(I)$	every 100 reflections
$R_{\text{int}} = 0.023$	intensity decay: none

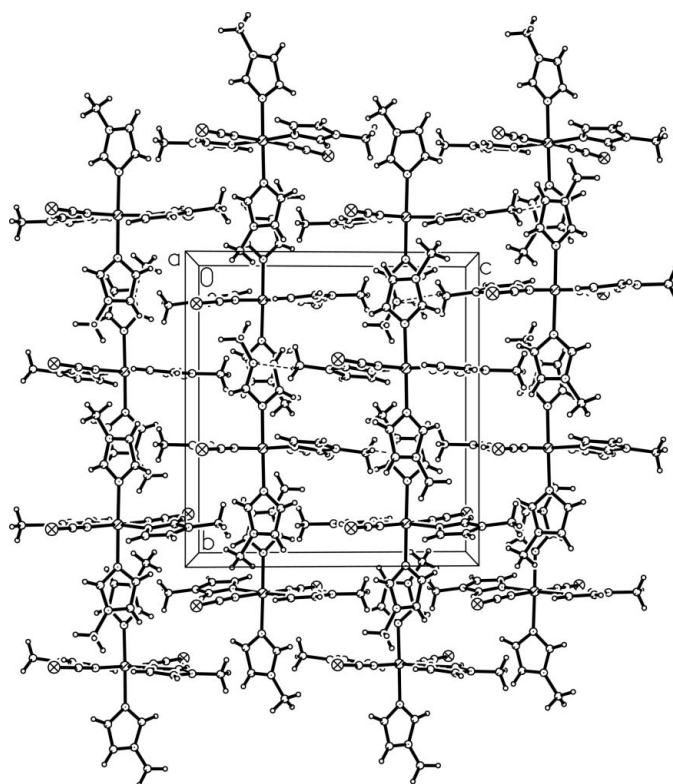


Figure 2
The packing of the title compound, viewed down the a axis.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 3.586P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.162$	$(\Delta/\sigma)_{\text{max}} = 0.004$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.81 \text{ e \AA}^{-3}$
5188 reflections	$\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$
285 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0007 (2)

Table 1

Selected geometric parameters (Å, °).

Ni1–N10	2.083 (4)	Ni1–N6	2.129 (4)
Ni1–N9	2.091 (4)	S1–C17	1.635 (5)
Ni1–N4	2.103 (4)	S2–C18	1.632 (5)
Ni1–N8	2.112 (4)	N9–C17	1.133 (6)
Ni1–N2	2.116 (4)	N10–C18	1.148 (6)
N10–Ni1–N9	178.63 (17)	N8–Ni1–N2	89.33 (15)
N10–Ni1–N4	90.26 (15)	N10–Ni1–N6	88.39 (16)
N9–Ni1–N4	90.40 (15)	N9–Ni1–N6	90.39 (16)
N10–Ni1–N8	89.51 (15)	N4–Ni1–N6	91.51 (15)
N9–Ni1–N8	89.87 (15)	N8–Ni1–N6	90.68 (15)
N4–Ni1–N8	177.80 (15)	N2–Ni1–N6	178.74 (15)
N10–Ni1–N2	90.35 (17)	N9–C17–S1	178.9 (5)
N9–Ni1–N2	90.87 (17)	N10–C18–S2	179.7 (5)
N4–Ni1–N2	88.48 (14)		

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C–H = 0.93–0.96 Å and $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*,

1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Natural Science Foundation of Shandong Province (grant No. Y2002B06) and the Science Research Foundation of Qingdao University of Science and Technology (grant No. 03Z08).

References

- Brooks, P. & Davidson, N. (1960). *J. Am. Chem. Soc.* **82**, 2118–2123.
- Davis, W. J. & Smith, J. (1971). *J. Chem. Soc. A*, pp. 317–324.
- Eilbeck, W. J., Holmes, F. & Underhill, A. E. (1967). *J. Chem. Soc. A*, pp. 757–761.
- Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Gabe, E. J., Le Page, Y., Charland, J. P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
- Koman, M., Jóna, E. & Māsejová, A. (1991). *Acta Cryst.* **C47**, 1206–1208.
- Liu, F.-Q., Jian, F.-F., Lu, L.-D., Yang, X.-J., Wang, X. & Xiao, H.-L. (2005). *Acta Cryst.* **E61**, m425–m426.
- Masejova, A., Uhrinova, S., Mrozinski, J., Zurowska, B., Munoz, M. C. & Julve, M. (1997). *Inorg. Chim. Acta*, **255**, 343–349.
- Sheldrick, G. M. (1990). *SHELXTL-PC*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.