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Tetrakis(1-ethyl-1*H*-imidazole-κN^3)diisothiocyanatonickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.073
wR factor = 0.198
Data-to-parameter ratio = 17.1

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

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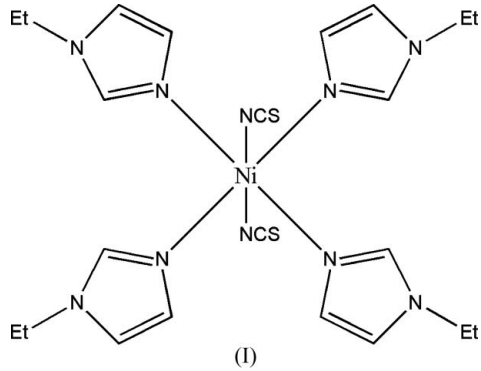
The structure of the title compound, $[Ni(NCS)_2(C_5H_8N_2)_4]$, consists of isolated molecules of $[Ni(NCS)_2(Eim)_4]$ (Eim = 1-ethylimidazole), which contain a compressed octahedral NiN_6 chromophore. The NCS^- anions are *trans* and four N atoms from the Eim ligands define the equatorial plane. The mean Ni—N(Eim) and Ni—N(NCS) distances are 2.117 (6) and 2.112 (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 possess diverse pharmacological effects, including anti-inflammatory, antimalarial and antitumor activities (Eilbeck *et al.*, 1967; Davis & Smith, 1971). The isothiocyanate anion is a versatile inorganic ligand in the synthesis of coordination compounds. It therefore seemed 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 stoichiometry of the resulting species (Maslejova, *et al.*, 1997). We have previously reported the crystal structures of Co(2-methylimidazole)$_2$(NCS)$_2$ (Liu, Jian, Lu *et al.*, 2005) and $[Ni(NCS)_2$(1-methylimidazole)$_4]$ (Liu, Jian, Liu *et al.*, 2005). In this paper, we report the crystal structure of tetrakis(1-ethyl-1*H*-imidazole-κN^3)diisothiocyanatonickel(II), (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Ni atom displays an octahedral coordination geometry, with six N atoms from two thiocyanate anions and four 1-ethylimidazole (Eim) ligands. The equatorial plane of the complex is formed by four Ni—N(Eim) bonds, with lengths ranging from

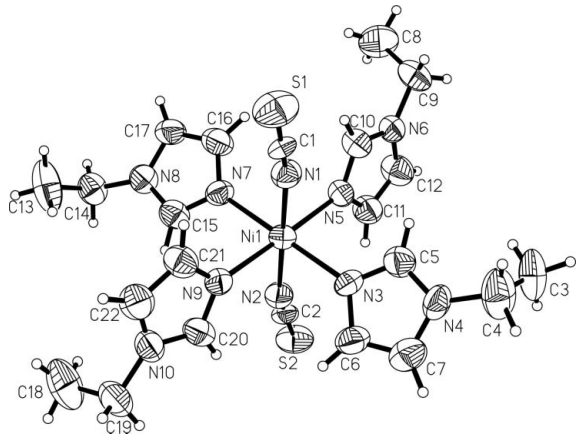


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

2.100 (6) to 2.131 (5) Å, and the axial positions are occupied by two N-bonded NCS groups [Ni—N(NCS) = 2.109 (4) and 2.115 (4) Å]. These values agree well with those observed in $[Ni(NCS)_2(Mim)_4]$ (Liu, Jian, Liu *et al.*, 2005). 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 N3—Ni1—N9 [93.02 (19)°]. The thiocyanate ligands are almost linear (Table 1).

Experimental

The title compound was prepared by the reaction of 1-ethylimidazole (1.92 g, 20 mmol) with $NiCl_2{\cdot}6H_2O$ (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

$[Ni(NCS)_2(C_5H_8N_2)_4]$
M_r = 559.41
Triclinic, $P\overline{1}$
a = 8.936 (2) Å
b = 13.186 (3) Å
c = 13.261 (3) Å
α = 72.16 (3)°
β = 89.20 (3)°
γ = 71.12 (3)°
V = 1401.1 (7) Å^3
Z = 2
D_x = 1.326 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 293 (2) K
Block, blue
0.35 × 0.25 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
5517 measured reflections
5495 independent reflections
3462 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 26.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.198
S = 1.06
5495 reflections
321 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1373P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.044 (5)

Table 1
Selected geometric parameters (Å, °).

Ni1—N3	2.100 (6)	Ni1—N7	2.131 (5)
Ni1—N1	2.109 (4)	S1—C1	1.638 (5)
Ni1—N5	2.115 (4)	S2—C2	1.631 (5)
Ni1—N2	2.115 (4)	N1—C1	1.147 (6)
Ni1—N9	2.121 (4)	N2—C2	1.151 (6)
N3—Ni1—N1	91.2 (2)	N5—Ni1—N9	178.5 (2)
N3—Ni1—N5	88.46 (19)	N2—Ni1—N9	89.56 (16)
N1—Ni1—N5	89.09 (16)	N3—Ni1—N7	178.56 (14)
N3—Ni1—N2	88.9 (2)	N1—Ni1—N7	89.8 (2)
N1—Ni1—N2	179.8 (2)	N5—Ni1—N7	90.56 (19)
N5—Ni1—N2	90.82 (16)	N2—Ni1—N7	90.0 (2)
N3—Ni1—N9	93.02 (19)	N9—Ni1—N7	87.97 (19)
N1—Ni1—N9	90.53 (16)		

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

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