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{2-(2-Pyridyl)-5-[(2-pyridylmethylidene)aminomethyl]-1,3-oxazoline-κ^4N}bis(thiocyanato-κN)nickel(II)

Hai-Ying Fu, Jian-Min Dou,* Da-Cheng Li and Da-Qi Wang

School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: jmdou@lcu.edu.cn

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The title complex, $[Ni(NCS)_2(C_{15}H_{16}N_4O)]$, consists of nickel(II) coordinated by 2-(2-pyridyl)-5-[(2-pyridylmethylidene)-aminomethyl]-1,3-oxazoline (*L*) and two *N*-coordinated thiocyanate ions. The coordination environment is NiN_6 distorted octahedral. Intermolecular N—H···S hydrogen bonds link adjacent $[Ni(SCN)_2(L)]$ molecules, forming a linear tape. In the synthesis, a five-membered ring has been formed by a nucleophilic addition reaction.

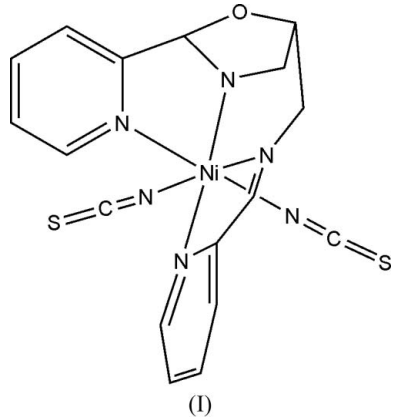
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.013 Å
R factor = 0.056
wR factor = 0.164
Data-to-parameter ratio = 14.0

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

Comment

In recent years, there has been considerable interest in metal complexes produced by the Schiff base condensation of 1,3-diamino-2-hydroxypropane with two equivalents of aromatic aldehyde or aromatic ketone due to their magnetochemistry and biological model chemistry (Bouchra *et al.*, 1986; Gajda *et al.*, 2002). Research on nickel complexes has been limited and only a few have been synthesized, such as $[Ni_2(C_{29}H_{47}N_8O)(H_2O)](ClO_4)_3$ (Mochizuki *et al.*, 2004), $[Ni_2(C_{29}H_{47}N_8O)(N_3)][(N_3)_2]\cdot 7H_2O$ (Mochizuki *et al.*, 2004), $[Ni(C_{13}H_{18}N_6O)(H_2O)_2][(ClO_4)_2]$ (Long *et al.*, 1999) and $[Ni(C_{18}H_{25}N_6S_2)](ClO_4)$ (Dipesh *et al.*, 2003). In our current work, we have synthesized the complex $[Ni(NCS)_2(C_{15}H_{16}N_4O)(NCS)_2]$, (I), whose structure is shown in Fig. 1.



(I)

The complex consists of one 2-(2-pyridyl)-5-[(2-pyridylmethylidene)aminomethyl]-1,3-oxazoline (*L*) ligand, one nickel(II) ion and two thiocyanate ions. The geometry around the nickel center can be described as distorted octahedral (Table 1) with an average Ni—N distance of 2.086 (6) Å.

As shown in Fig. 2, adjacent $[Ni(SCN)_2(L)]$ molecules are linked by N2—H2···S1^{i} [symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$] hydrogen bonds, with an N2···S1^{i} distance of 3.390 Å, forming a one-dimensional zigzag chain.

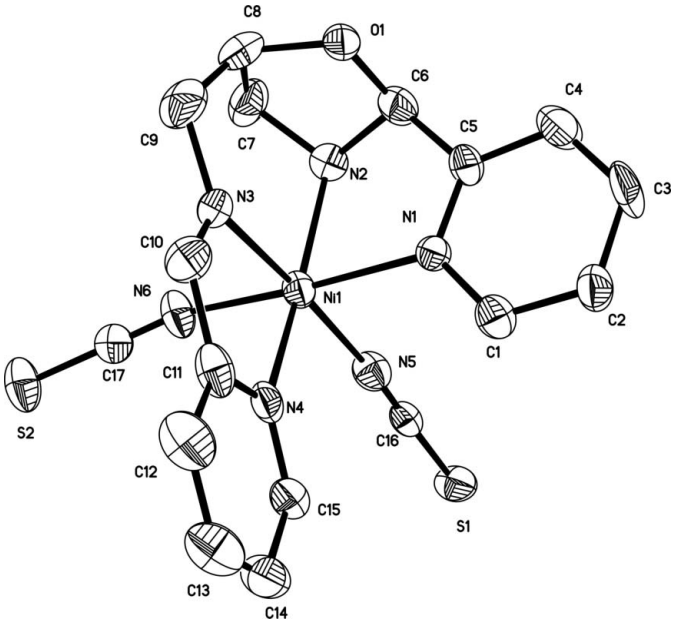


Figure 1
The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

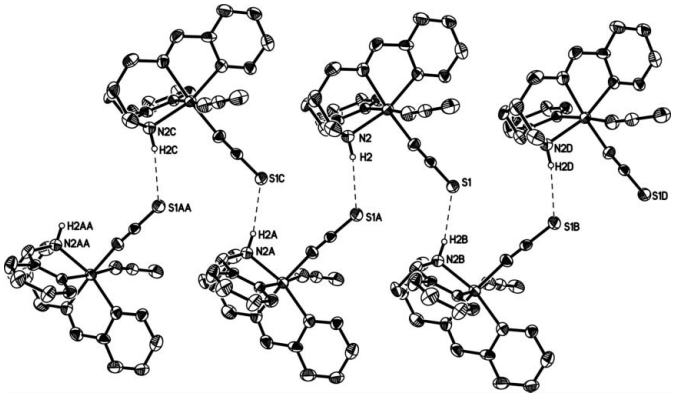


Figure 2
The one-dimensional chain formed by hydrogen-bond interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

The five-membered ring is formed by the nucleophilic addition reaction between the C═N double bond and the propanol hydroxy group in the ligand.

Experimental

To a stirred solution of 1,3-diamino-2-propanol (0.09 g, 1 mmol) in 6 ml of dry methanol was added 2-pyridinecarboxaldehyde (0.214 g, 2 mmol) in 6 ml of dry methanol. The stirred mixture was refluxed for 2 h to afford a methanol solution of ligand *L*. Ligand *L* (1 mmol, 0.268 g) in methanol and $Ni(SCN)_2$ (1 mmol, 0.175 g) in methanol were mixed. The solution was stirred at room temperature for about 4 h and later a red–brown precipitate formed. The precipitate was dissolved in dimethylformamide. About a week later, red crystals were isolated from the solution [m.p. 542–543 K (decomposition)].

Crystal data

$[Ni(NCS)_2(C_{15}H_{16}N_4O)]$
M_r = 443.19
Orthorhombic, $P2_12_12_1$
a = 8.524 (5) Å
b = 15.044 (9) Å
c = 15.218 (9) Å
V = 1951.4 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.23 mm^{-1}
T = 298 (2) K
0.33 × 0.31 × 0.29 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.687, T_{max} = 0.717
9991 measured reflections
3427 independent reflections
2429 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.164
S = 1.00
3427 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.02 (3)

Table 1
Selected geometric parameters (Å, °).

Ni1—N6	2.058 (7)	Ni1—N1	2.099 (6)
Ni1—N5	2.061 (7)	Ni1—N2	2.104 (6)
Ni1—N4	2.079 (7)	Ni1—N3	2.114 (6)
N6—Ni1—N5	91.6 (3)	N4—Ni1—N2	164.4 (2)
N6—Ni1—N4	91.8 (3)	N1—Ni1—N2	79.2 (2)
N5—Ni1—N4	95.9 (3)	N6—Ni1—N3	88.6 (3)
N6—Ni1—N1	175.2 (3)	N5—Ni1—N3	174.8 (3)
N5—Ni1—N1	88.0 (2)	N4—Ni1—N3	78.9 (3)
N4—Ni1—N1	92.9 (2)	N1—Ni1—N3	92.2 (2)
N6—Ni1—N2	96.1 (3)	N2—Ni1—N3	87.9 (3)
N5—Ni1—N2	97.2 (3)		

All H atoms were positioned geometrically and treated as riding on their parent atoms, with benzene C—H distances of 0.93 Å, methylene C—H distances of 0.97 Å, methine C—H distances of 0.98 or 0.93 Å and amino N—H distances of 0.91Å. The U_{iso}(H) values were set at 1.2U_{eq}(C) for all C-bound H atoms and at 1.2U_{eq}(N) for all N-bound H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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