

## Guang Chen

Department of Chemistry, Qufu Normal  
University, Qufu 273165, People's Republic  
of ChinaCorrespondence e-mail:  
qufuchenguang@163.com

## Key indicators

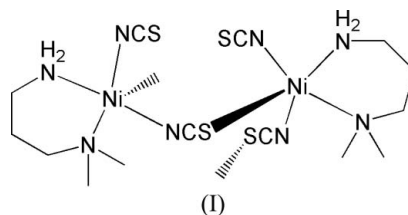
Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.067  
Data-to-parameter ratio = 19.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**catena-Poly[[*N,N*-dimethylpropane-1,3-diamine)-  
thiocyanatonickel(II)]- $\mu$ -thiocyanato]**

The title compound,  $[\text{Ni}(\text{NCS})_2(\text{C}_5\text{H}_{14}\text{N}_2)]_n$ , is a thiocyanate-bridged polynuclear nickel(II) complex. The Ni atom is five-coordinated in a square-pyramidal geometry, with two N atoms of the *N,N*-dimethylpropane-1,3-diamine ligand and two N atoms from two thiocyanate ligands defining the basal plane, and one S atom of another thiocyanate ligand occupying the apical position. The  $[\text{Ni}(\text{NCS})_2(\text{C}_5\text{H}_{14}\text{N}_2)]$  units are linked by bridging thiocyanate ligands, forming chains running along the *b* axis.

Received 13 November 2006  
Accepted 20 November 2006

## Comment

Recently, we have reported the structures of a few transition metal complexes (Chen *et al.*, 2004*a,b*, 2005). As an extension of the work on the structural characterization of nickel compounds, the title compound, (I), is reported here.



Compound (I) is a thiocyanate-bridged polynuclear nickel(II) complex (Fig. 1). The Ni atom is five-coordinated in a square-pyramidal geometry, with two N atoms of the *N,N*-dimethylpropane-1,3-diamine ligand and two N atoms from two thiocyanate ligands defining the basal plane, and one S atom of another thiocyanate ligand occupying the apical position. The significant distortion of the square pyramid is revealed by the bond angles between the apical and basal donor atoms (Table 1). The bond lengths related to the metal atom are typical and comparable to the values in other nickel(II) complexes (Ariyananda & Norman, 2006*a,b*; Moore & Norman, 2006). In the crystal structure, molecules are linked by bridging thiocyanate ligands, forming polymeric chains running along the *b* axis.

## Experimental

*N,N*-Dimethylpropane-1,3-diamine (1.0 mmol, 102.2 mg), NaNCS (1.0 mmol, 81.1 mg), and  $\text{Ni}(\text{ClO}_4)_2 \cdot 7\text{H}_2\text{O}$  (1.0 mmol, 383.7 mg) were dissolved in a methanol solution (50 ml). The mixture was stirred for 1 h at room temperature and then filtered. After keeping the green filtrate in air for one week, green plate-shaped crystals were formed.

Crystal data

[Ni(NCS)<sub>2</sub>(C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>)]

*M<sub>r</sub>* = 277.05

Monoclinic, *P*<sub>2</sub><sub>1</sub>

*a* = 8.216 (1) Å

*b* = 6.927 (1) Å

*c* = 10.987 (2) Å

β = 110.819 (2)°

*V* = 584.47 (15) Å<sup>3</sup>

*Z* = 2

*D<sub>x</sub>* = 1.574 Mg m<sup>-3</sup>

Mo *K*α radiation

μ = 1.99 mm<sup>-1</sup>

*T* = 298 (2) K

Plate, green

0.35 × 0.11 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

*T<sub>min</sub>* = 0.543, *T<sub>max</sub>* = 0.925

4931 measured reflections

2542 independent reflections

2376 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.027

θ<sub>max</sub> = 27.5°

Refinement

Refinement on *F*<sup>2</sup>

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.029

*wR*(*F*<sup>2</sup>) = 0.067

*S* = 1.03

2542 reflections

130 parameters

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0252*P*)<sup>2</sup>]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/*σ*)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 0.31 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.25 e Å<sup>-3</sup>

Absolute structure: Flack (1983),

1118 Friedel pairs

Flack parameter: 0.576 (14)

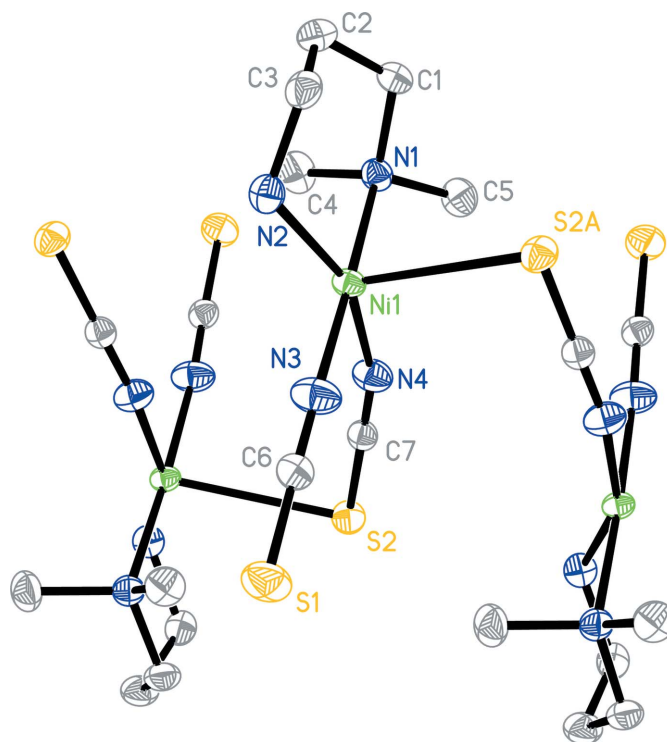


Figure 1

Part of the polymeric structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The atom labelled with the suffix A is at the symmetry position  $(-x, -\frac{1}{2} + y, 2 - z)$ . H atoms have been omitted.

Table 1

Selected geometric parameters (Å, °).

Ni1—N1	2.073 (3)	Ni1—N4	1.961 (3)
Ni1—N2	1.993 (3)	Ni1—S2 <sup>i</sup>	2.8439 (10)
Ni1—N3	1.968 (3)		
N4—Ni1—N3	87.64 (12)	N2—Ni1—N1	92.44 (11)
N4—Ni1—N2	156.87 (15)	N1—Ni1—S2 <sup>i</sup>	90.86 (11)
N3—Ni1—N2	88.24 (14)	N2—Ni1—S2 <sup>i</sup>	97.92 (11)
N4—Ni1—N1	90.78 (12)	N3—Ni1—S2 <sup>i</sup>	91.49 (11)
N3—Ni1—N1	177.4 (2)	N4—Ni1—S2 <sup>i</sup>	104.93 (11)

Symmetry code: (i)  $-x, y - \frac{1}{2}, -z + 2$ .

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2 <i>B</i> ...S2 <sup>ii</sup>	0.90	2.58	3.473 (4)	171
N2—H2 <i>A</i> ...S2 <sup>iii</sup>	0.90	2.73	3.586 (4)	159

Symmetry codes: (ii)  $x + 1, y, z$ ; (iii)  $-x, y + \frac{1}{2}, -z + 2$ .

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.96–0.97 Å and N—H distances of 0.90 Å. They were treated as riding atoms, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C,N) or 1.5*U*<sub>eq</sub>(C). The value of the Flack (1983) parameter is indicative of inversion twinning in the crystal.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve

structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The author thanks Qufu Normal University for the research grant No. xj03005.

References

- Ariyananda, W. G. P. & Norman, R. E. (2006a). *Acta Cryst.* E62, m2336–m2338.
- Ariyananda, W. G. P. & Norman, R. E. (2006b). *Acta Cryst.* E62, m2339–m2341.
- Chen, G., Bai, Z.-P. & Qu, S.-J. (2005). *Acta Cryst.* E61, m2718–m2719.
- Chen, G., Sun, Y.-X., Sun, M. & Qi, W. (2004a). *Acta Cryst.* E60, m1547–m1549.
- Chen, G., Sun, Y.-X., Sun, M. & Qi, W. (2004b). *Acta Cryst.* E60, m1550–m1551.
- Flack, H. D. (1983). *Acta Cryst.* A39, 876–881.
- Moore, L. E. Jr & Norman, R. E. (2006). *Acta Cryst.* E62, m2342–m2344.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). SHELXL97 and SHELXS97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.