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## Key indicators

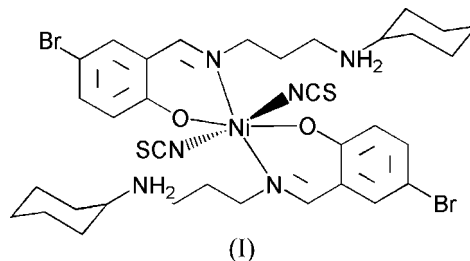
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$   
 $R$  factor = 0.080  
 $wR$  factor = 0.154  
Data-to-parameter ratio = 19.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis{4-bromo-2-[3-(cyclohexylamino)propyl-  
iminomethyl]phenolato}dithiocyanatonickel(II)

In the title compound,  $[\text{Ni}(\text{NCS})_2(\text{C}_{16}\text{H}_{23}\text{BrN}_2\text{O})_2]$ , the Ni atom lies on an inversion centre; it is chelated by the phenolate O and imine N atoms from two Schiff base ligands, and is coordinated by the N atoms from two thiocyanate ligands, giving a slightly distorted octahedral geometry. In the crystal structure, molecules form chains running along the  $a$  axis *via* intermolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds.

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## Comment

Nickel(II) complexes derived from Schiff base ligands have received much attention in coordination chemistry related to catalysis and enzymatic reactions, magnetism and coordination diversity (Di Bella *et al.*, 1994; Lacroix *et al.*, 1996; Averseng *et al.*, 1999; Wang, 2005; Fun *et al.*, 2001; Zhang *et al.*, 2005). As a further investigation of the structures of such complexes, the title compound, (I), a new mononuclear nickel(II) complex, is reported here.



In compound (I), the Ni atom lies on an inversion centre; it is chelated by the phenolate O and imine N atoms from two

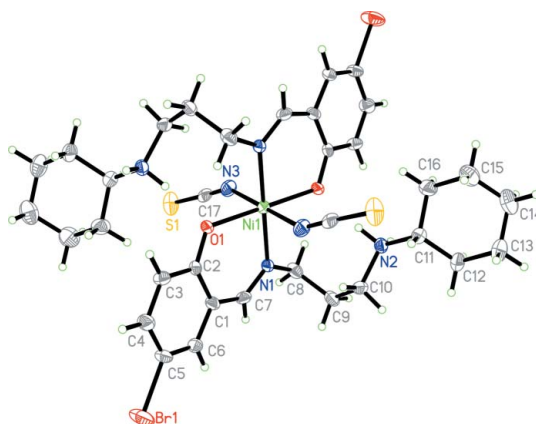
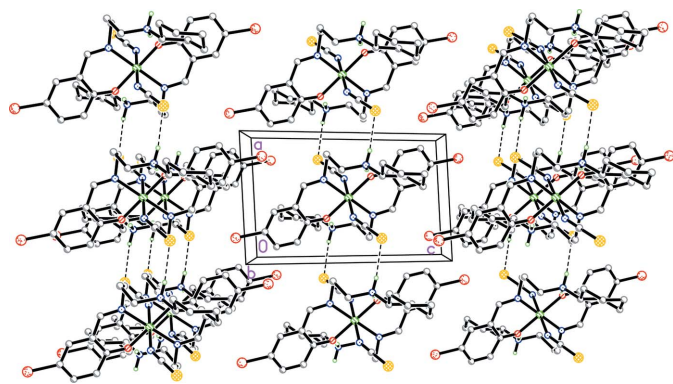


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position  $(1-x, 1-y, 1-z)$ .



**Figure 2**  
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines.

Schiff base ligands, and is coordinated by the N atoms from two thiocyanate ligands (Fig. 1). While the three *trans* angles at Ni are 180° by symmetry, the other angles are close to 90°, ranging from 86.6 (2) to 93.4 (2)° (Table 1), indicating a slightly distorted octahedral coordination. The Ni—O and Ni—N bond lengths are typical (Table 1) and are comparable with those observed in other similar nickel(II) complexes (Wei, 2005; Ali *et al.*, 2004; Sari *et al.*, 2006; Gomes *et al.*, 2000). The amine N atom of the pendant propylaminocyclohexyl unit is protonated and takes no part in the coordination to the Ni atom.

In the crystal structure, molecules of (I) are linked *via* intermolecular N—H···O and N—H···S hydrogen bonds (Table 2), forming chains running along the *a* axis (Fig. 2).

### Experimental

5-Bromosalicylaldehyde (1.0 mmol, 202.3 mg), *N*-cyclohexyl-1,3-diaminopropane (1.0 mmol, 156.1 mg), ammonium thiocyanate (1.0 mmol, 76.2 mg) and Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (0.5 mmol, 145.3 mg) were dissolved in MeOH (50 ml). The mixture was stirred at room temperature for about 1 h to give a green solution. After keeping the solution in air for a week, small green block-like crystals of (I) were formed.

#### Crystal data

[Ni(NCS) <sub>2</sub> (C <sub>16</sub> H <sub>23</sub> BrN <sub>2</sub> O) <sub>2</sub> ]	<i>V</i> = 987.0 (4) Å <sup>3</sup>
<i>M<sub>r</sub></i> = 853.42	<i>Z</i> = 1
Triclinic, <i>P</i> $\bar{1}$	<i>D<sub>x</sub></i> = 1.436 Mg m <sup>-3</sup>
<i>a</i> = 7.623 (2) Å	Mo <i>K</i> α radiation
<i>b</i> = 10.732 (2) Å	<i>μ</i> = 2.66 mm <sup>-1</sup>
<i>c</i> = 13.036 (3) Å	<i>T</i> = 298 (2) K
<i>α</i> = 112.089 (4)°	Block, green
<i>β</i> = 92.535 (4)°	0.09 × 0.06 × 0.02 mm
<i>γ</i> = 90.422 (4)°	

#### Data collection

Bruker SMART CCD area-detector diffractometer	8527 measured reflections
<i>ω</i> scans	4360 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	1995 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T<sub>min</sub></i> = 0.796, <i>T<sub>max</sub></i> = 0.949	<i>R<sub>int</sub></i> = 0.089
	<i>θ<sub>max</sub></i> = 27.5°

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.081  
*wR*(*F*<sup>2</sup>) = 0.154  
*S* = 0.96  
 4360 reflections  
 220 parameters

H atoms treated by a mixture of independent and constrained refinement  
*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.037*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> = 0.52 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.42 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ni1—O1	2.023 (4)	Ni1—N3	2.120 (6)
Ni1—N1	2.072 (5)		
O1 <sup>i</sup> —Ni1—O1	180	N1—Ni1—N3 <sup>i</sup>	93.4 (2)
O1—Ni1—N1 <sup>i</sup>	90.83 (18)	O1—Ni1—N3	89.0 (2)
O1—Ni1—N1	89.17 (17)	N1—Ni1—N3	86.6 (2)
N1 <sup>i</sup> —Ni1—N1	180	N3 <sup>i</sup> —Ni1—N3	180
O1—Ni1—N3 <sup>i</sup>	91.0 (2)		

Symmetry code: (i) -*x* + 1, -*y* + 1, -*z* + 1.

**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—H2A···O1 <sup>i</sup>	0.91 (5)	1.79 (5)	2.697 (7)	173 (6)
N2—H2B···S1 <sup>ii</sup>	0.91 (3)	2.402 (15)	3.296 (6)	171 (6)

Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z* + 1; (ii) -*x*, -*y* + 1, -*z* + 1.

The H atoms bound to N2 were located in a difference Fourier map and refined isotropically, with N—H and H···H distances restrained to 0.90 (1) Å and 1.43 (2) Å, respectively. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C). The ratio of observed to unique reflections is low (46%), as is the fraction of reflections measured (96.5%), due to the poor diffraction quality of the crystal. The structure contains solvent-accessible voids of 88 Å<sup>3</sup>, which might accommodate a disordered water molecule.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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