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#### Key indicators

Single-crystal X-ray study  
 $T = 200$  K  
 Mean  $\sigma(C-C) = 0.017$  Å  
 Disorder in main residue  
 $R$  factor = 0.075  
 $wR$  factor = 0.245  
 Data-to-parameter ratio = 13.8

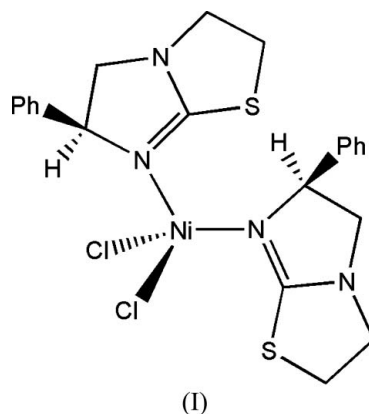
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Dichlorobis[(*S*)-2,3,5,6-tetrahydro-6-phenylimidazo[2,1-*b*]thiazole]nickel(II)

The title compound,  $[\text{NiCl}_2(\text{C}_{11}\text{H}_{12}\text{N}_2\text{S})_2]$ , crystallizes with two independent molecules per asymmetric unit. The Ni atom displays a pseudo-tetrahedral environment of the ligands, as expected for paramagnetic  $\text{Ni}^{\text{II}}$  compounds.

#### Comment

Levamisole (lvms), (*S*)-2,3,5,6-tetrahydro-6-phenylimidazo[2,1-*b*]thiazole, and levamisole hydrochloride are well known anthelmintic drugs with immunomodulatory (Amery & Bruynseels, 1992) and anticancer (Kovach *et al.*, 1992) activities. However, very few inorganic derivatives of levamisole have been reported: the only examples to date are the mononuclear complexes  $[\text{MCl}_2(\text{lvms})_2]$  ( $M = \text{Co}, \text{Ni}, \text{Cu}$  or  $\text{Zn}$ ; Kovachev *et al.*, 1994),  $[\text{Pd}(\eta^2\text{-aminoacidato})(\text{lvms})_2]\text{Cl}$  (Nijasure *et al.*, 1999) and  $[\text{PtCl}(\text{en})(\text{lvms})]\text{Cl}$  (en is ethylenediamine; Arvanitis *et al.*, 1993). A trinuclear derivative,  $[\text{Ru}_3(\mu\text{-Cl})(\mu\text{-}\eta^2\text{-C}_{11}\text{H}_{13}\text{N}_2\text{S-C,S})(\text{CO})_9]$ , was also reported by Cabeza *et al.* (2002). The ligand of this last complex arises from a C–S bond cleavage of levamisole hydrochloride. To date, only the structures of the last two complexes have been determined by X-ray diffraction methods. We report here the structure of the title compound, (I), a compound previously described by the Stoychkov group (Kovachev *et al.*, 1994), which has some activity as an immunomodulating drug.



The structures of the two independent chiral molecules of  $[\text{NiCl}_2(\text{lvms})_2]$ , (I), are illustrated in Fig. 1. The compound crystallizes in the monoclinic space group  $P2_1$ , with two independent molecules in the asymmetric unit. The coordination environment of the Ni atom is nearly tetrahedral. Both levamisole ligands bind to the metal atom through their  $sp^2$ -hybridized N atom. The two crystallographically independent molecules show two different conformations of the title compound.

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## Experimental

Compound (I) was synthesized as previously described by Kovachev *et al.* (1994). Crystallization was accomplished from an acetone–diethyl ether solution (1:2 v/v) at room temperature by slow liquid–liquid diffusion.

### Crystal data

[NiCl<sub>2</sub>(C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>S)<sub>2</sub>]

*M<sub>r</sub>* = 538.19

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

*a* = 8.1791 (5) Å

*b* = 9.2534 (4) Å

*c* = 31.556 (2) Å

β = 91.637 (3)°

*V* = 2387.3 (2) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.497 Mg m<sup>-3</sup>

Cu Kα radiation

Cell parameters from 4366

reflections

θ = 1.4–69.6°

μ = 5.00 mm<sup>-1</sup>

*T* = 200 (2) K

Plate, blue

0.18 × 0.18 × 0.03 mm

### Data collection

Nonius KappaCCD area-detector diffractometer

φ and ω scans

Absorption correction: refined on Δ*F* (*XABS2*; Parkin *et al.*, 1995)

*T<sub>min</sub>* = 0.476, *T<sub>max</sub>* = 0.866

7693 measured reflections

7693 independent reflections

6015 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.061

θ<sub>max</sub> = 69.6°

*h* = −9 → 9

*k* = −11 → 9

*l* = −38 → 38

### Refinement

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

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.076

*wR*(*F*<sup>2</sup>) = 0.245

*S* = 1.18

7693 reflections

559 parameters

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.1088*P*)<sup>2</sup> + 6.3761*P*]

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> = 0.91 e Å<sup>-3</sup>

Δρ<sub>min</sub> = −0.77 e Å<sup>-3</sup>

Extinction correction: *SHELXL97*

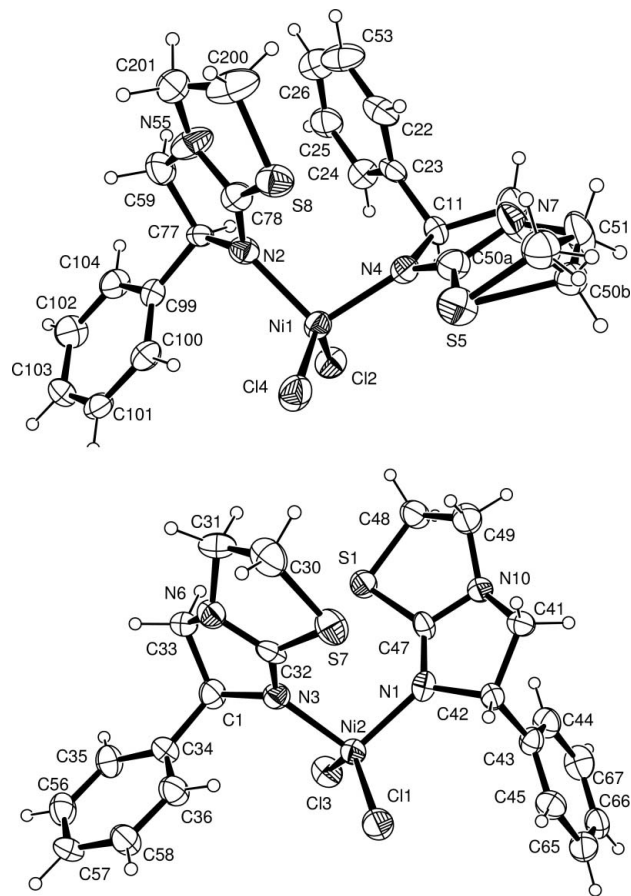
(Sheldrick, 1997)

Extinction coefficient: 0.0016 (3)

Absolute structure: Flack (1983),

2930 Friedel pairs

Flack parameter: 0.02 (4)



**Figure 1**

The two independent molecules of (I) in the asymmetric unit, showing 50% probability displacement ellipsoids.

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