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 Ni\(^{II}\) 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 \([\text{MCl}_2(\text{lvms})_2]\) \((\text{M} = \text{Co}, \text{Ni}, \text{Cu} \text{or Zn}; \text{Kovachev et al.}, 1994), [\text{Pd}(\eta^5\text{-aminoacidato})(\text{lvms})_2]\text{Cl} \text{(Nijasure et al., 1999)} \text{and [PtCl}(\text{en})(\text{lvms})\text{Cl (en is ethylenediamine; Arvanitis et al., 1993). A trinuclear derivative, [Ru}_3(\mu-\text{Cl})(\mu- \eta^2\text{-C}_1\text{H}_2\text{N}_2\text{S})_3\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.
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

\[[\text{NiCl}_2(\text{C}_\text{11}\text{H}_\text{12}\text{N}_\text{2}\text{S})_2]\]

- \( M_r = 538.19 \)
- Monoclinic, \( P2_1 \)
- \( a = 8.1791 (5) \) Å
- \( b = 9.2534 (4) \) Å
- \( c = 31.556 (2) \) Å
- \( \beta = 91.637 (3) ^\circ \)
- \( V = 2387.3 (2) \) Å³
- \( Z = 4 \)

- \( D_x = 1.497 \) Mg m⁻³
- Cu \( K\alpha \) radiation

Cell parameters from 4366 reflections
- \( \theta = 1.4–49.6^\circ \)
- \( \mu = 5.00 \) mm⁻¹
- \( T = 200 (2) \) K
- Plate, blue

0.18 × 0.18 × 0.03 mm

Data collection

Nonius KappaCCD area-detector diffractometer
- \( \varphi \) and \( \omega \) scans
- Absorption correction: refined on \( \Delta F(XABS2; Parkin et al., 1995) \)
- \( \theta_{\text{max}} = 0.476, \theta_{\text{max}} = 0.866 \)
- 7693 measured reflections

Refinement

Refinement on \( F^2 \)
- \( R[F^2 > 2\sigma(F^2)] = 0.076 \)
- \( wR(F^2) = 0.245 \)
- \( S = 1.18 \)
- 7693 independent reflections

559 parameters
- H-atom parameters constrained
- \( w = 1/\sigma^2(F^2) + (0.1088P)^2 + 6.3761P \)

where \( P = (F^2 + 2F^2)/3 \)

\( \Delta\rho_{\text{max}} = 0.001 \)
- \( \Delta\rho_{\text{min}} = -0.77 \) e Å⁻³

Extinction correction: \( \text{SHELXL97} \)

Extinction coefficient: 0.0016 (3)
- Absolute structure: Flack (1983), 50% probability displacement ellipsoids.
- 2930 Friedel pairs
- Flack parameter: 0.02 (4)

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References


