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

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Key indicators

Single-crystal X-ray study
T = 200 K
Mean σ(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.

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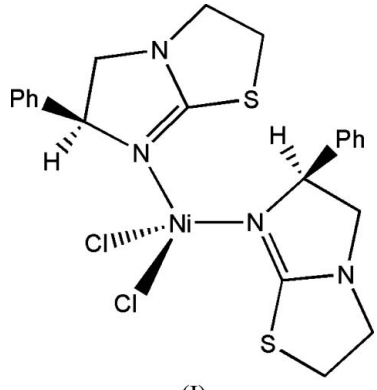
The title compound, $[NiCl_2(C_{11}H_{12}N_2S)_2]$, crystallizes with two independent molecules per asymmetric unit. The Ni atom displays a pseudo-tetrahedral environment of the ligands, as expected for paramagnetic Ni^{II} compounds.

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 $[MCl_2(lvms)_2]$ (*M* = Co, Ni, Cu or Zn; Kovachev *et al.*, 1994), [Pd(η^2-aminoacidato)$(lvms)_2$]Cl (Nijasure *et al.*, 1999) and [PtCl(en)(lvms)]Cl (en is ethylendiamine; Arvanitis *et al.*, 1993). A trinuclear derivative, $[Ru_3(\mu\text{-Cl})(\mu\text{-}\eta^2\text{-}C_{11}H_{13}N_2S\text{-}C,S)(CO)_9]$, 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.



(I)

The structures of the two independent chiral molecules of $[NiCl_2(lvms)_2]$, (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

$[NiCl_2(C_{11}H_{12}N_2S)_2]$	D_x = 1.497 Mg m^{-3}
M_r = 538.19	Cu $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 4366 reflections
a = 8.1791 (5) Å	θ = 1.4–69.6°
b = 9.2534 (4) Å	μ = 5.00 mm^{-1}
c = 31.556 (2) Å	T = 200 (2) K
β = 91.637 (3)°	Plate, blue
V = 2387.3 (2) Å^3	0.18 × 0.18 × 0.03 mm
Z = 4	

Data collection

Nonius KappaCCD area-detector diffractometer	7693 independent reflections
φ and ω scans	6015 reflections with $I > 2\sigma(I)$
Absorption correction: refined on ΔF (*XABS2*; Parkin *et al.*, 1995)	R_{int} = 0.061
T_{min} = 0.476, T_{max} = 0.866	θ_{max} = 69.6°
7693 measured reflections	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 9$
	$l = -38 \rightarrow 38$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max}$ = 0.001
$R[F^2 > 2\sigma(F^2)]$ = 0.076	$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$wR(F^2)$ = 0.245	$\Delta\rho_{min}$ = −0.77 e Å^{-3}
S = 1.18	Extinction correction: *SHELXL97* (Sheldrick, 1997)
7693 reflections	Extinction coefficient: 0.0016 (3)
559 parameters	Absolute structure: Flack (1983), 2930 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.02 (4)
$w = 1/[\sigma^2(F_o^2) + (0.1088P)^2 + 6.3761P]$ where $P = (F_o^2 + 2F_c^2)/3$	

All H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.98 Å. They were included in the refinement in a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atom. Atom C50 was found to be disordered between two alternative sites, C50*A* and C50*B*, with occupancies of 70% and 30%, respectively; the occupancies were initially refined but were fixed in the final stages of refinement. The split atomic positions for C50 were refined isotropically.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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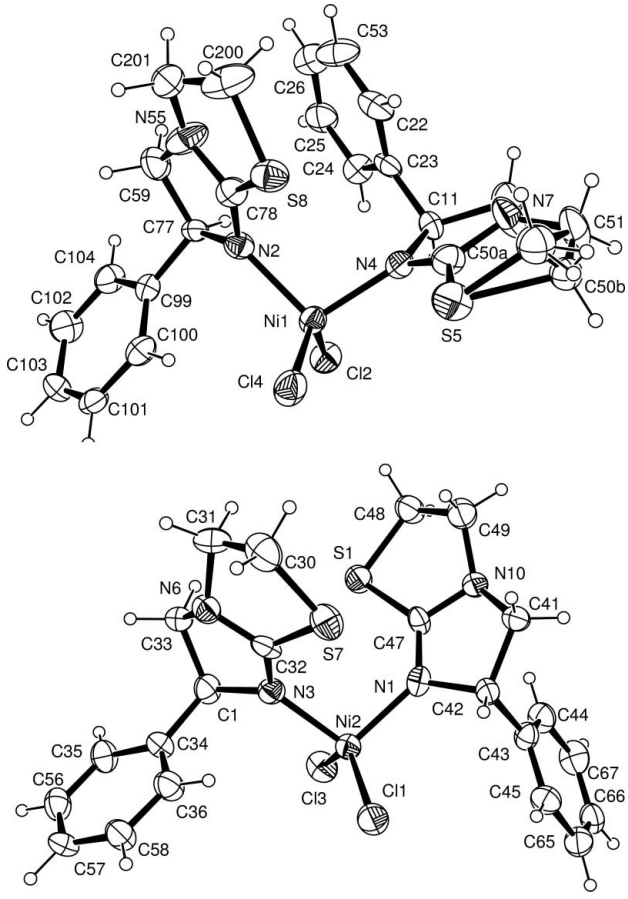

Figure 1
The two independent molecules of (I) in the asymmetric unit, showing 50% probability displacement ellipsoids.

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