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Dichlorobis(1,2-phenylenediamine)-nickel(II)

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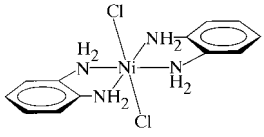
The title compound, $[NiCl_2(C_6H_8N_2)_2]$, contains centrosymmetric molecules with two phenylenediamine ligands coordinated in a bidentate fashion. The Ni—N distances are 2.088 (1) and 2.096 (1) Å, and the Ni—Cl distance of 2.4635 (4) Å. The plane of each phenylenediamine molecule makes a dihedral angle of 26.53 (7)° with the NiN_4 plane. Extensive hydrogen bonding leads to distinct cleavage in the *bc* plane.

Comment

The title compound, (I), was prepared for use as a starting material in the synthesis of Haldane Gap systems (Haldane, 1983). The latter can be realised by linear-chain systems of antiferromagnetically coupled $S = 1$ species.



(I)

Experimental

The title compound was prepared by the reaction of 1,2-phenylenediamine dihydrochloride (0.989 g, 5.46 mmol) with $NiCl_2{\cdot}6H_2O$ (0.386 g, 2.00 mmol) in water (30 ml) under a nitrogen atmosphere for 5 d. The solution was then stored in a sealed tube at room temperature. After 8 d, brown rod-shaped crystals had formed. They were removed by filtration and washed with cold water.

Crystal data

$[NiCl_2(C_6H_8N_2)_2]$	$D_x = 1.546$ Mg m^{-3}
$M_r = 345.90$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4572 reflections
$a = 11.3793$ (2) Å	$\theta = 1.98$–$28.19°$
$b = 5.9240$ (1) Å	$\mu = 1.656$ mm^{-1}
$c = 12.1901$ (1) Å	$T = 213$ (2) K
$\beta = 115.31°$	Block, green
$V = 742.841$ (19) Å^3	0.35 × 0.20 × 0.15 mm
$Z = 2$	

Data collection

CCD diffractometer	$R_{int} = 0.022$
ω scans	$\theta_{max} = 28.19°$
Absorption correction: empirical (*SADABS*; Bruker, 1997)	$h = -15 \rightarrow 10$
$T_{min} = 0.650$, $T_{max} = 0.780$	$k = -7 \rightarrow 7$
4572 measured reflections	$l = -15 \rightarrow 16$
1758 independent reflections	50 frames standard reflections
1702 reflections with $I > 2\sigma(I)$	frequency: beginning and end
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0134P)^2 + 0.3976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R(F) = 0.023$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.057$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.218$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1758 reflections	Extinction correction: *SHELXL*97
121 parameters	Extinction coefficient: 0.0137 (12)
All H-atom parameters refined	

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The use of the single-crystal diffraction facility in the Office of Research at the University of Idaho is appreciated.

References

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