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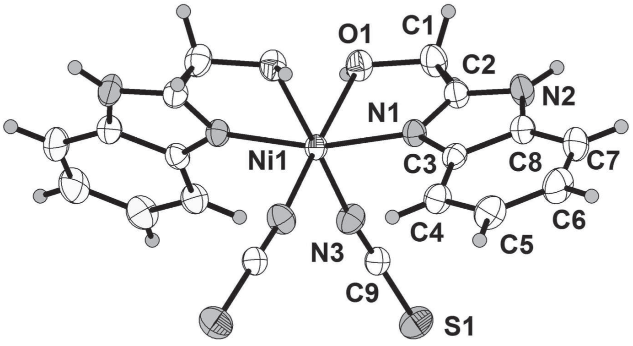
Crystal structure of cis-bis((1*H*-benzimidazol-2-yl) methanol-κ*N*,*O*)-bis(isothiocyanato-κ*N*)nickel(II), $C_{18}H_{16}N_6NiO_2S_2$



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Abstract

$C_{18}H_{16}N_6NiO_2S_2$, monoclinic, $C2/c$ (no. 15), $a = 14.935(3)$ Å, $b = 8.5054(17)$ Å, $c = 16.268(3)$ Å, $\beta = 109.45(3)°$, $V = 1948.5(8)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0243$, $wR_{ref}(F^2) = 0.0669$, $T = 293(2)$ K.

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The title complex located on a twofold axis in its crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Dark-green block
Size:	0.20 × 0.20 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	12.4 cm^{-1}
Diffractometer, scan mode:	Bruker APEXII, φ and ω
$2\theta_{max}$, completeness:	57°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8603, 2443, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2298
$N(param)_{refined}$:	132
Programs:	Bruker programs [1, 2], SHELX [3], DIAMOND [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	$U_{iso}*/U_{eq}$
Ni1	0.0000	0.77628(3)	0.2500	0.02415(8)
S1	0.24516(3)	0.38414(5)	0.31948(3)	0.03853(11)
O1	0.10748(7)	0.95944(13)	0.27971(6)	0.0340(2)
H1C	0.1425	0.9402	0.2514	0.041*
N1	0.03078(8)	0.80851(13)	0.38138(7)	0.0273(2)
C3	−0.00078(10)	0.75616(15)	0.44834(9)	0.0276(3)
N3	0.10503(9)	0.61567(15)	0.26822(8)	0.0354(3)
C9	0.16352(9)	0.52175(16)	0.28858(8)	0.0285(3)
N2	0.12697(9)	0.90409(16)	0.50627(8)	0.0371(3)
H2	0.1736	0.9547	0.5421	0.045*
C4	−0.07681(10)	0.66094(18)	0.44675(10)	.0338(3)
H4	−0.1174	0.6194	0.3948	0.041*
C7	0.04749(13)	0.7832(2)	0.60690(10)	0.0437(4)
H7	0.0888	0.8223	0.6592	0.052*
C1	0.16229(10)	0.97039(19)	0.36954(10)	0.0373(3)
H1A	0.1750	1.0796	0.3865	0.045*
H1B	0.2224	0.9163	0.3811	0.045*
C2	0.10579(10)	0.89560(16)	0.41918(9)	0.0309(3)
C5	−0.08975(12)	0.6303(2)	0.52544(11)	0.0419(3)
H5	−0.1407	0.5681	0.5262	0.050*
C8	0.05962(10)	0.81615(17)	0.52738(9)	0.0331(3)
C6	−0.02833(13)	0.6903(2)	0.60404(11)	0.0468(4)
H6	−0.0393	0.6666	0.6557	0.056*

Source of material

All reagents and solvents employed were commercially available and used as received without further purification.

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$NiCl_2·6H_2O$ (0.5 mmol, 0.119 g), 1*H*-benzimidazole-2-methanol (1 mmol, 0.148 g) and KSCN (1 mmol, 0.098 g) in acetonitrile (8 mL) and methanol (8 mL) were reacted. After addition of tetramethylammonium hydroxide (0.2 mmol, 25% in water) the mixture was heated and then stirred for 12h and filtered. Evaporation of the filtrate under ambient conditions afforded dark-green block-shaped crystals in a yield of 45%.

Experimental details

All the non-H atoms were refined anisotropically. H atoms were subsequently treated as riding atoms with distances C—H = 0.96 (CH_3), 0.97 (CH_2), 0.93 Å (ArH) and O—H = 0.85 Å.

Discussion

Single-molecule magnets (SMMs) have attracted considerable interest [5–8]. The majority of SMMs characterised to date have contained the metal manganese [9]. SMMs containing Ni(II) ions are far less common despite the fact that mononuclear nickel complexes have been shown to possess |D| values greater than 10 cm^{-1} [10]. Only a limited number of Ni(II) SMMs were reported [11]. In order to enlarge the knowledge on nickel(II) complexs, the 1*H*-benzimidazole-2-methanol ligand was selected for the synthesis of nickel(II) coordination compounds due to its different coordination modes. The asymmetric unit contains one half of a title complex located on a twofold axis of the space group *C*2/*c*.

The hexacoordinate Ni(II) coordination environment is composed of two nitrogen atoms of two crystallographically related 1*H*-benzimidazole-2-methanol ligands with a Ni(1)–N(1) bond length 2.049 Å. The two crystallographically related hydroxy groups of the aforementioned organic ligand show a Ni(1)–O(1) bond length of 2.173 Å. The thiocyanate Ni(1)-N(3) bond length is 2.026 Å. The Ni1(II) ion displays distorted octahedral coordination environment, with the N(1), O(1), N(1A), N(3) forming the basal plane and the N(3A), O(1A) occupying the axial position. The deviation of the nickel atom is 0.133 Å from the basal plane. Hydrogen bonds play an important role for the interactions between the adjacent complexes.

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