Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(1,1′-butane-1,4-diyldiimidazole-κN^3)nickel(II)]-μ-1,1′-butane-1,4-diyldiimidazole-$\kappa^2N^3:N^{3'}$], a one-dimensional coordination polymer

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Received 3 January 2006
Accepted 9 January 2006

Key indicators

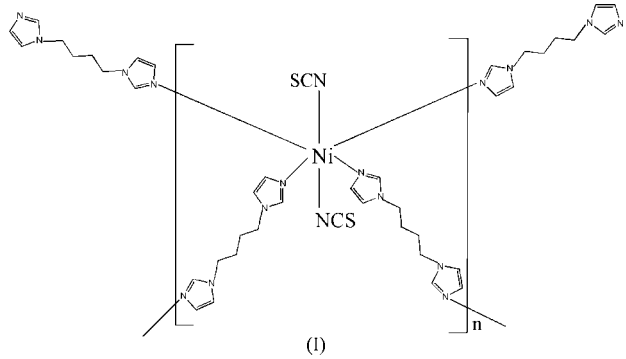
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.083
Data-to-parameter ratio = 13.7

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

In the title compound, $[Ni(NCS)_2(C_{10}H_{14}N_4)_2]_n$, the Ni^{II} ion (site symmetry $\bar{1}$) is coordinated by six N atoms from four different 1,1′-butane-1,4-diyldiimidazole ligands and two SCN^- anions, in a slightly distorted octahedral geometry. Adjacent Ni^{II} ions are linked by pairs of 1,1′-butane-1,4-diyldiimidazole molecules, resulting in a one-dimensional polymeric structure with a double-strand chain.

Comment

The preparation of metal–organic coordination polymers with novel topologies has attracted great interest from chemists, due to their potential applications as functional solid materials, as well as their fascinating framework structures (Eddaoudi *et al.*, 2001). 4,4′-Byridine is a rigid rod-like spacer, well known in the construction of metal–organic polymers, and it has adopted numerous interesting supramolecular architectures (Batten & Robson, 1998). However, flexible ligands such as 1,1′-(1,4-butanediyl)bis(imidazole) (*L*) have not been so well explored to date (Ma *et al.*, 2003). In this work, the combination of *L* with Ni^{II} cations and thiocyanate anions resulted in the title compound, (I), an interesting one-dimensional coordination polymer with a double-strand chain.



(I)

Selected bond lengths and angles for (I) are given in Table 1. The Ni^{II} ion (site symmetry $\bar{1}$) is six-coordinated by six N atoms from four different *L* ligands and two SCN^- anions, in a distorted octahedral geometry (Fig. 1). The average Ni—N (*L*) distance is 2.123 (2) Å, which is similar to that observed in $[Ni(L')(N_3)_2]\cdot 2H_2O$ [*L*′ is 1,3,5-tris(1-imidazolyl)benzene; Fan *et al.*, 2003]. It is noteworthy that, in (I), only the N atoms of the SCN^- anions coordinate to the metal centre, while in the related compound $[Co(SCN)_2(bim)]$ [bim is 1,2-bis(imidazol-1-yl)ethane], the S atoms are also connected to the central metal atom (Wang *et al.*, 2005).

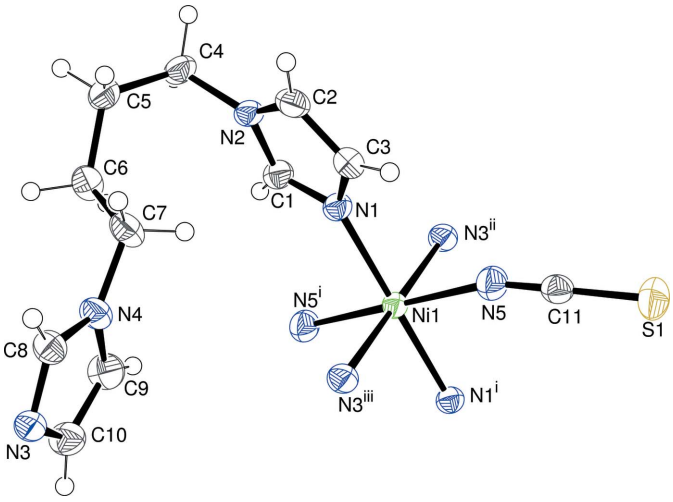


Figure 1
Detail of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $x-1, y, z$; (iii) $2-x, -y, 1-z$.]

The polymeric connectivity in (I) results in two strands of the *L* ligands wrapped around each other, held together by Ni^{II} ions to form a double-strand chain (Fig. 2). The intrachain Ni···Ni separation is equal to the *a* axis translation distance of 8.9269 (4) Å, which is shorter than the Zn···Zn separation of 10.851 Å in the related compound $Zn(L)(ClO_4)_2$ (Cui *et al.*, 2005).

There are no supramolecular interactions, such as hydrogen bonds or π–π stacking forces, in the structure of (I). The packing is shown in Fig. 3.

Experimental

The *L* ligand was synthesized according to the literature method of Yang *et al.* (2005). A methanolic solution (10 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (10 ml) of $NiCl_2{\cdot}H_2O$ (0.5 mmol) and KSCN (1 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several days, yielding pale-blue crystals of (I) (65% yield based on Ni).

Crystal data

$[Ni(NCS)_2(C_{10}H_{14}N_4)_2]$
$M_r = 555.37$
Monoclinic, $P2_1/c$
$a = 8.9269$ (4) Å
$b = 9.6590$ (5) Å
$c = 14.4390$ (8) Å
$\beta = 91.073$ (4)°
$V = 1244.78$ (11) Å^3
$Z = 2$
$D_x = 1.482$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6670 reflections
$\theta = 2.3$–25°
$\mu = 0.98$ mm^{-1}
$T = 292$ (2) K
Block, light blue
0.35 × 0.29 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.704$, $T_{max} = 0.760$
6670 measured reflections
2197 independent reflections
1766 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 25.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 10$
$l = -11 \rightarrow 17$

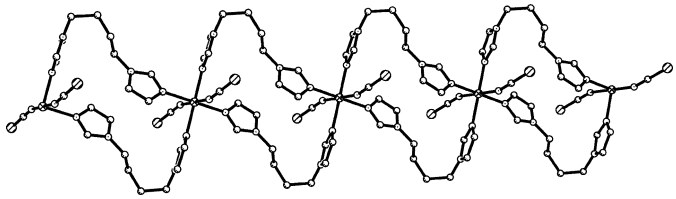


Figure 2
The double-strand chain structure of (I). H atoms have been omitted.

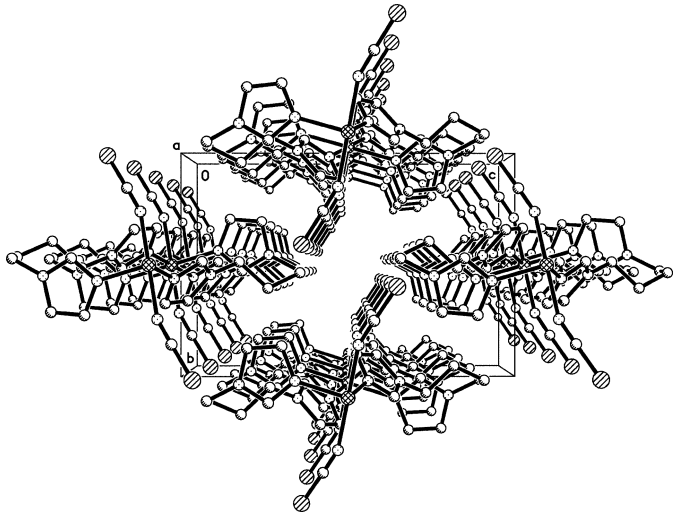


Figure 3
The packing structure of (I). H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.083$
$S = 1.03$
2197 reflections
160 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N5	2.096 (2)	Ni1—N3^{i}	2.134 (2)
Ni1—N1	2.1113 (19)		
Ni1—N5—C11	159.0 (2)		

Symmetry code: (i) $x-1, y, z$.

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL*.

The authors thank Jilin Normal University for supporting this work.

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