

Poly[μ -cyano- μ -pyrazine-nickel(I)]

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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.009$ Å
 R factor = 0.040
 wR factor = 0.116
Data-to-parameter ratio = 11.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

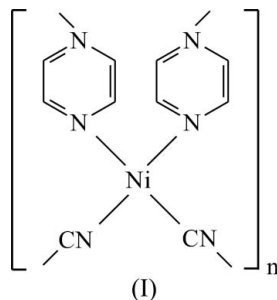
The title compound, $[\text{Ni}(\text{CN})(\text{C}_4\text{H}_4\text{N}_2)]_n$, was prepared by the hydrothermal reaction of NiCl_2 , KCN and pyrazine. The Ni^{II} atoms are linked *via* cyanide ligands into a zigzag $[\text{NC}-\text{Ni}-\text{NC}]_\infty$ chain running parallel to $[010]$. These chains are further connected into a three-dimensional network by bridging pyrazine ligands, which have inversion symmetry. The coordination geometry around the Ni^{II} atom is distorted tetrahedral, with one N and one C atom from the cyanide and two N atoms from the pyrazine ligands.

Received 28 July 2006
Accepted 4 August 2006

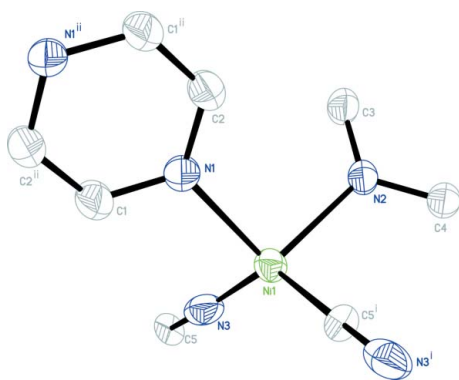
Comment

The design of cyanide-bridged compounds has been the subject of long-lasting research interest, not only because of their appealing structural and topological novelty, but also due to their unusual optical, electronic, magnetic and catalytic properties (Mironov *et al.*, 2003; Boudalis *et al.*, 2004; Berlinguette *et al.*, 2003; Sokol *et al.*, 2002; Soler *et al.*, 2004). In such complexes, cyanide ligands play a major role in the ability to facilitate long-range electron transfer and to mediate magnetic exchange interactions (Klausmeyer & Rauchfuss, 1998; Marvilliers *et al.*, 1999; Oshio *et al.*, 2000; Parker *et al.*, 2001; Ferlay *et al.*, 1995; Sato *et al.*, 1996). In addition, cyanide ligands generally form extraordinarily stable complexes that allow for the construction of two- and three-dimensional arrays of cyanide-based coordination units (Ferlay *et al.*, 1995; Sato *et al.*, 1996; Pilkington & Decurtins, 2000).

Recently, versatile organic building blocks have been introduced to control the dimensionality of desired complexes with novel magnetic properties; this is a new strategy in



assembling cyanide-bridged complexes of the form $[\text{M}(\text{L})_x(\text{CN})_y]^{n-}$ (M is a first row transition metal and L is a blocking ligand). So far, a variety of structures with cyano-bridged complexes, including molecular clusters (Sokol *et al.*, 2001; Oshio *et al.*, 2003; Wang *et al.*, 2004; Kim *et al.*, 2004), one-dimensional chains (Toma *et al.*, 2004; Matsumoto *et al.*, 1999), and two-dimensional layered networks (Lescouzec *et al.*, 2001, 2004), have been synthesized. This indicates that


Figure 1

A view of the local geometry around Ni in the structure of (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $\frac{1}{2} + x, \frac{3}{2} - y, z - \frac{1}{2}$; (ii) $\frac{1}{2} + x, \frac{3}{2} - y, z + \frac{1}{2}$]

organic building blocks seem very promising in designing novel cyano-bridged complexes with desired structures and/or magnetic properties, especially low-dimensional hetero-bimetallic systems. We report here the synthesis and structure analysis of the title compound, (I).

In compound (I), the Ni atom is tetrahedrally coordinated by three N atoms from one cyanide and two pyrazine ligands, and by one cyanide C atom (Fig. 1). The geometry around Ni is considerably distorted (Table 1), with Ni–N(pyrazine) bond lengths of 2.131 (5) and 2.150 (5) Å, and a much shorter Ni–N(cyanide) bond length of 1.962 (7) Å. At 1.901 (5) Å, the Ni–C(cyanide) distance is the shortest.

If the pyrazine ligands are neglected, one-dimensional zigzag [CN–Ni–NC] $_{\infty}$ chains running parallel to [010] are formed, which is shown in the packing diagram of (I) in Fig. 2.

Experimental

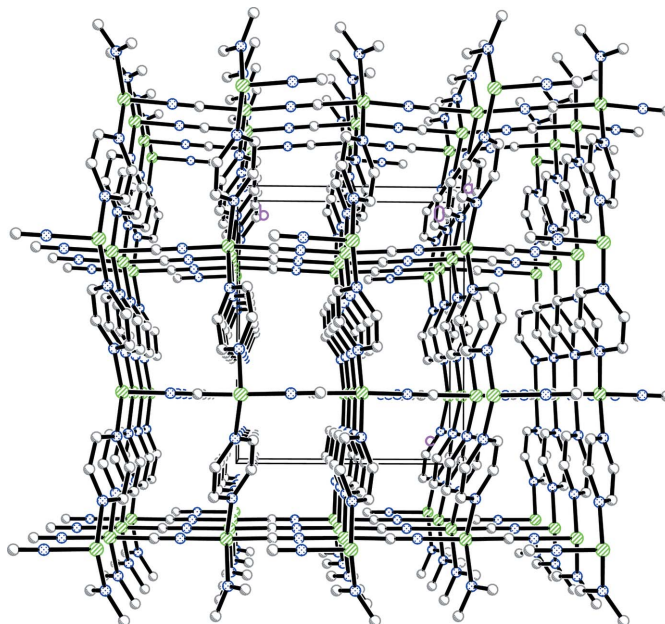
For the synthesis of (I), analytical grade reagents (99%) were employed. A mixture of NiCl $_2$ ·6H $_2$ O (0.5 mmol), KCN (0.5 mmol), pyrazine (1 mmol) and H $_2$ O (8 ml) was heated at 443 K for 2 d in a 25 ml Teflon-lined stainless steel autoclave, and then cooled to room temperature. Green crystals of (I) were obtained in a yield of 35%. Analysis calculated for C $_5$ H $_4$ N $_3$ Ni: C 36.41, H 2.43, N 25.49, Ni 35.61%; found: C 36.40, H 2.41, N 25.31, Ni 35.52%.

Crystal data

[Ni(CN)(C $_4$ H $_4$ N $_2$)]	Z = 4
$M_r = 164.82$	$D_x = 1.730 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.193 (3) \text{ \AA}$	$\mu = 2.96 \text{ mm}^{-1}$
$b = 9.152 (4) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 11.167 (5) \text{ \AA}$	Block, green
$\beta = 90.908 (5)^\circ$	$0.20 \times 0.20 \times 0.20 \text{ mm}$
$V = 632.9 (5) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	3130 measured reflections
φ and ω scans	1110 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	803 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.589, T_{\max} = 0.589$	$R_{\text{int}} = 0.034$
(expected range = 0.553–0.553)	$\theta_{\text{max}} = 25.0^\circ$


Figure 2

A packing diagram of (I), viewed along the a axis. Ni atoms are represented by green hatched spheres, N atoms by blue dotted spheres and C atoms by grey-lined spheres. H atoms have been omitted for clarity.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 1.4011P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.116$	$(\Delta/\sigma)_{\text{max}} = 0.009$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$
1110 reflections	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$
98 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

N1–C1	1.320 (8)	N3–C5	1.107 (7)
N1–C2	1.325 (7)	C1–C2 ⁱ	1.362 (9)
N2–C4	1.328 (8)	C3–C4 ⁱⁱ	1.357 (9)
N2–C3	1.334 (8)		
C5 ⁱⁱⁱ –Ni1–N3	133.2 (2)	C5 ⁱⁱⁱ –Ni1–N1	101.2 (2)
C5 ⁱⁱⁱ –Ni1–N2	99.3 (2)	N3–Ni1–N1	106.47 (19)
N3–Ni1–N2	111.90 (19)	N2–Ni1–N1	99.99 (19)
Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$			

H atoms were located in difference density maps and refined isotropically with bond-distance restraints [C1–H1 = 0.98 (4) Å, C2–H2 = 0.98 (4) Å, C3–H3 = 0.93 (4) Å and C4–H4 = 1.00 (4) Å].

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXL97.

The authors thank Liaocheng Natural Science Foundation (grant No. 20501011) and Liaocheng University (grant No. 31801) for financial support. In addition, we thank Professor Jianmin Dou for his help.

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