Poly[(μ-4-methylpyridine N-oxide)bis(μ-thio-cyanato)cobalt(II)]

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In the title complex, $[Co(\mu\text{-}NCS)_2(\mu\text{-}C_6H_7NO)]_n$, both the thiocyanate and 4-methylpyridine N-oxide ligands coordinate to the Co^{II} atom as bridging ligands, forming a two-dimensional sheet structure. There is a non-classical C—H···S hydrogen bond in the sheet.

Comment

Both thiocyanate and pyridine N-oxide are very useful bridging ligands. A number of multinuclear complexes have been synthesized with one or both of them as bridging ligands and some of the complexes display interesting physical properties (Shi, Sun et al., 2006). Interest in complexes containing both ligands resulted in the synthesis of the title complex, (I), and we report its structure here. The synthesis of (I) was almost identical to that of the one-dimensional polymer $[Co(\mu_{1,3}\text{-}SCN)(\mu\text{-}C_6H_7NO)(SCN)(CH_3OH)]_n$ (Shi, Liu et al., 2006), but the difference in the solvents led to the formation of the two complexes with distinct structures.

(I)
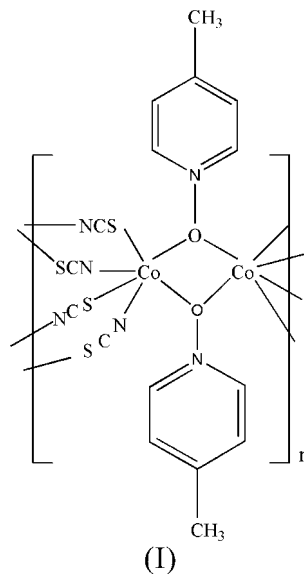
The Co^{II} atom assumes a distorted octahedral $CoO_2N_2S_2$ coordination geometry (Fig. 1 and Table 1). Two 4-methyl-pyridine N-oxide molecules coordinate to two symmetry-related Co^{II} ions, with a Co1···Co1[iii] separation of 3.4452 (14) Å (symmetry code as in Table 1), forming a binuclear four-membered ring. Adjacent pairs of Co^{II} atoms are connected by the coordination of two $\mu_{1,3}$-SCN bridging ligands, creating an eight-membered ring; the Co···Co distances are 5.657 (2) and 5.690 (2) Å for Co1···Co1[i] and Co1···Co1[ii], respectively (symmetry codes as in Table 1). In this complex, a two-dimensional sheet structure is formed
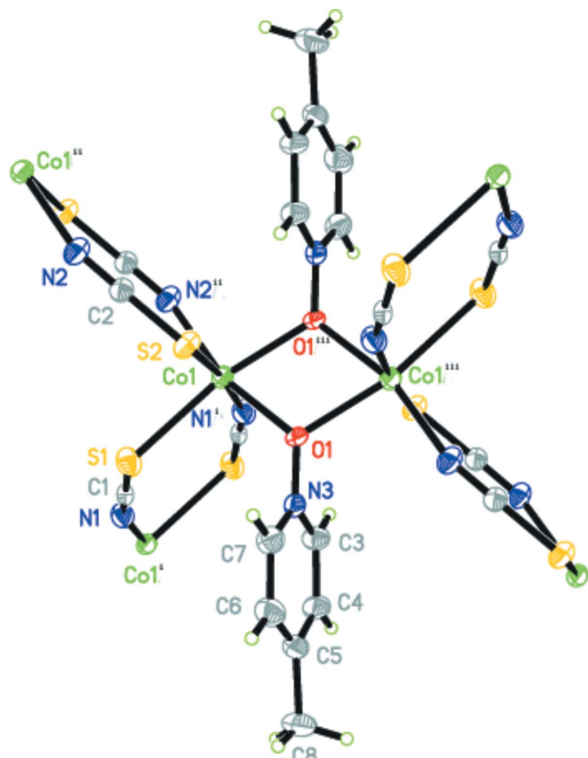
Figure 1
Part of the polymeric structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme (symmetry codes as in Table 1).
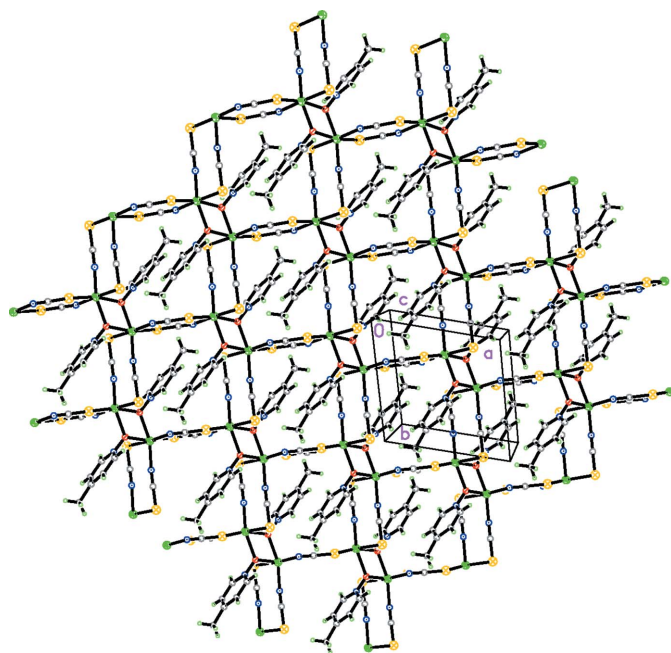

Figure 2
Packing diagram of (I), showing the two-dimensional sheet structure.

(Fig. 2). In the two-dimensional structure, there is a 34-membered ring formed by eight $\mu_{1,3}$-SCN bridging ligands, four μ-4-methylpyridine *N*-oxide ligands and six Co^{II} ions. A non-classical C—H$\cdots$S hydrogen bond (Table 2) is also observed in the sheet.

The 4-methoxypyridine analogue has been reported in a previous paper (Zhang *et al.*, 2006).

Experimental

Crystal data

[Co(NCS)$_2$(C$_6$H$_7$NO)]	$V = 558.5$ (3) Å^3
$M_r = 284.24$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.690$ Mg m^{-3}
$a = 7.945$ (3) Å	Mo $K\alpha$ radiation
$b = 8.170$ (3) Å	$\mu = 1.88$ mm^{-1}
$c = 9.642$ (3) Å	$T = 298$ (2) K
$\alpha = 71.059$ (5)°	Prism, blue
$\beta = 76.441$ (5)°	$0.46 \times 0.16 \times 0.08$ mm
$\gamma = 72.690$ (4)°	

Data collection

Bruker SMART APEX CCD diffractometer	2953 measured reflections
φ and ω scans	1981 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1419 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.478$, $T_{\max} = 0.864$	$R_{\mathrm{int}} = 0.049$
	$\theta_{\max} = 25.3°$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{\max} < 0.001$
1981 reflections	$\Delta\rho_{\max} = 0.51$ e Å^{-3}
137 parameters	$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N1^i	2.052 (4)	Co1—O1^{iii}	2.149 (3)
Co1—N2^{ii}	2.036 (4)	Co1—S1	2.5156 (16)
Co1—O1	2.097 (3)	Co1—S2	2.6500 (15)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1, -y+1, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H2$\cdots$S2^{iii}	0.93	2.86	3.590 (6)	137

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

H atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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