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Poly[(μ-4-methoxypyridine *N*-oxide)bis($\mu_{1,3}$-thiocyanato)cobalt(II)]: a two-dimensional coordination polymer

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.052
wR factor = 0.128
Data-to-parameter ratio = 14.5

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

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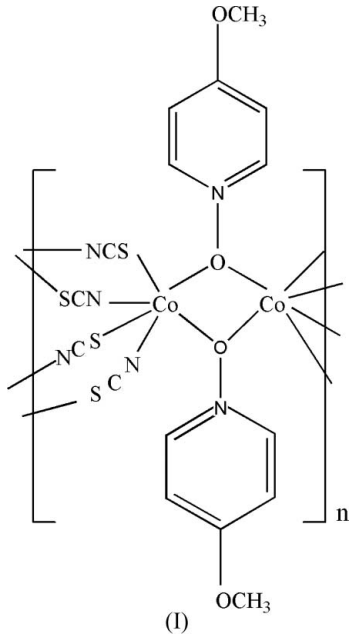
The title structure, $[Co(\mu\text{-}NCS)_2(\mu\text{-}C_6H_7NO_2)]_n$, forms two-dimensional sheets parallel to the *ab* plane in which both the thiocyanate and 4-methoxypyridine *N*-oxide ligands act as bridging ligands.

Comment

Thiocyanate and pyridine *N*-oxide (or its derivatives) are very useful bridging ligands and many coordination polymers (Shi, *et al.*, 2006) have been synthesized using these ligands. Some of these complexes display interesting magnetic properties. We are interested in compounds containing both types of ligand and hence we have synthesized the title complex, (I), whose crystal structure is reported here.



(I)

The asymmetric unit and symmetry-related fragments of (I) are shown in Fig. 1. Atom Co1 is in a distorted octahedral $CoO_2N_2S_2$ coordination geometry (Table 1). In the crystal structure, each Co^{II} atom is surrounded by three other symmetry-related Co^{II} atoms, with pairs of Co^{II} atoms connected through two $\mu_{1,3}$-SCN bridging ligands, with Co···Co separations of 5.660 (2) and 5.688 (2) Å, creating an eight-membered ring. Two 4-methoxypyridine *N*-oxide ligands bridge two other Co^{II} atoms, with a Co···Co separation of 3.4146 (14) Å, and form a binuclear four-membered ring with the four atoms strictly coplanar by virtue of the crystallographic inversion center which is at the middle of the four-membered ring. The overall structure of (I) is a two-dimen-

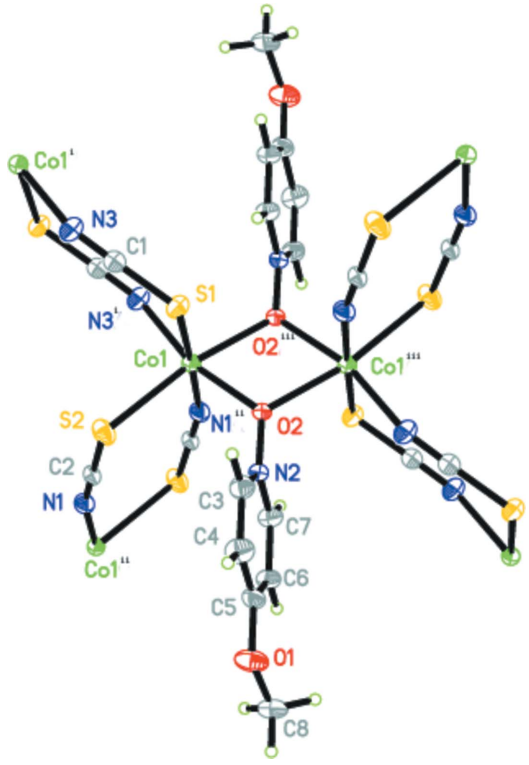


Figure 1
A portion of the two-dimensional structure of (I), showing the atom-numbering scheme with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$.]

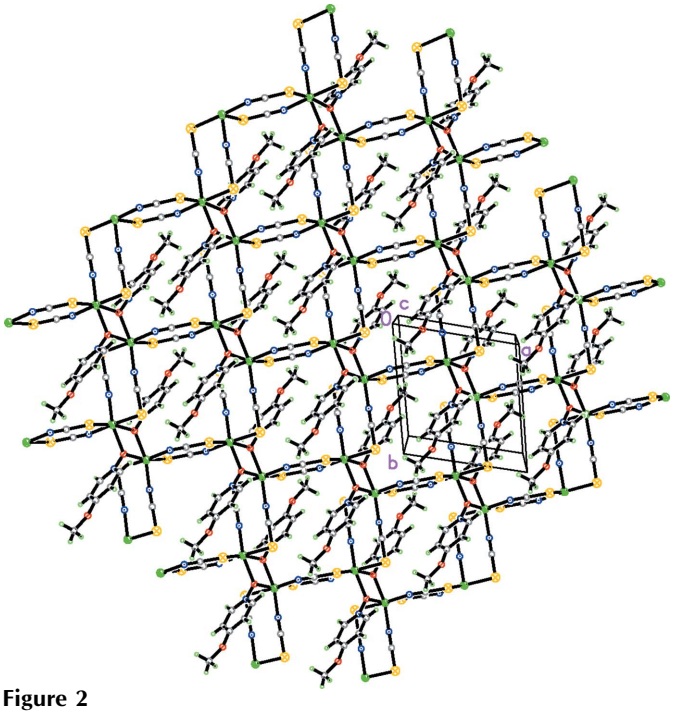


Figure 2
Part of the crystal structure of (I).

sional sheet parallel to the *ab* plane, as shown in Fig. 2. The crystal structure of (I) is very similar to that of the two-dimensional coordination polymer (μ-4-methylpyridine *N*-oxide)bis($\mu_{1,3}$-thiocyanato)cobalt(II); the different *para* substituents on the pyridine rings in the two structures do not appear to greatly affect the overall crystal packing.

Experimental

$Co(ClO_4)_2\cdot 6H_2O$ (0.2142 g, 0.585 mmol), 4-methoxypyridine *N*-oxide (0.0728 g, 0.582 mmol) and NaSCN (0.0945 g, 1.17 mmol) were separately dissolved in water (5 ml each), and then the three solutions were mixed together. Blue–purple single crystals of (I) were obtained after allowing the mixed solution to stand at room temperature for one month.

Crystal data

$[Co(NCS)_2(C_6H_7NO_2)]$
$M_r = 300.24$
Triclinic, $P\overline{1}$
$a = 7.884$ (3) Å
$b = 8.213$ (3) Å
$c = 9.860$ (3) Å
$\alpha = 75.319$ (5)°
$\beta = 74.170$ (4)°
$\gamma = 72.364$ (5)°
$V = 575.1$ (4) Å^3
$Z = 2$
$D_x = 1.734$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.84$ mm^{-1}
$T = 298$ (2) K
Prism, blue–purple
0.16 × 0.09 × 0.07 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.757$, $T_{max} = 0.882$
2995 measured reflections
2113 independent reflections
1697 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.128$
$S = 1.06$
2113 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N3^{i}	2.030 (4)	Co1—O2^{iii}	2.129 (3)
Co1—N1^{ii}	2.066 (4)	Co1—S2	2.5323 (15)
Co1—O2	2.086 (3)	Co1—S1	2.6369 (14)
N3^{i}—Co1—N1^{ii}	94.29 (16)	O2—Co1—S2	94.25 (9)
N3^{i}—Co1—O2	165.05 (14)	O2^{iii}—Co1—S2	165.52 (9)
N1^{ii}—Co1—O2	94.19 (14)	N3^{i}—Co1—S1	90.03 (12)
N3^{i}—Co1—O2^{iii}	95.56 (14)	N1^{ii}—Co1—S1	174.00 (11)
N1^{ii}—Co1—O2^{iii}	92.28 (14)	O2—Co1—S1	82.50 (9)
O2—Co1—O2^{iii}	71.81 (13)	O2^{iii}—Co1—S1	91.44 (9)
N3^{i}—Co1—S2	97.62 (12)	S2—Co1—S1	82.61 (5)
N1^{ii}—Co1—S2	92.67 (11)		

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

H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2_{eq}(C)$ for the pyridine ring, and C—H = 0.96 Å and $U_{iso}(H) = 1.5_{eq}(C)$ for the methyl group.

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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