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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.027
 wR factor = 0.069
Data-to-parameter ratio = 15.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquabis(3-hydroxypyridine *N*-oxide)-
dithiocyanatocobalt(II)

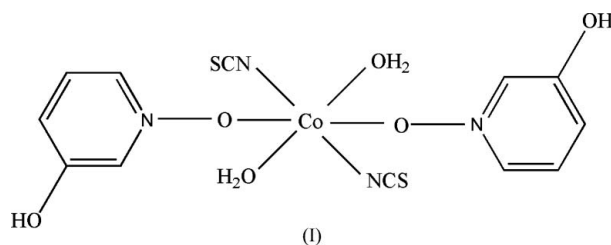
In the title mononuclear complex, $[\text{Co}(\text{NCS})_2(\text{C}_5\text{H}_5\text{NO}_2)_2(\text{H}_2\text{O})_2]$, the six-coordinated Co^{II} atom lies on an inversion center. In the crystal structure, intermolecular $\text{O}-\text{H}\cdots\text{O}$ ($\text{H}\cdots\text{O} = 1.85\text{--}2.01$ Å) and $\text{O}-\text{H}\cdots\text{S}$ ($\text{H}\cdots\text{S} = 2.40$ Å) hydrogen bonds link molecules into a three-dimensional network.

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Comment

We have recently determined the structures of two complexes which are related to the title compound, namely $[\text{Cu}_2(\mu_{1,3}\text{-SCN})_2(\mu'_{1,3}\text{-SCN})_2(\text{MPyO})_2]_n$ (where $\text{MPyO} = 4\text{-methylpyridine } N\text{-oxide}$) (Shi *et al.*, 2006) and diaquadiisothiocyanatobis(pyridine *N*-oxide)cobalt(II) (Shi *et al.*, 2005). In the title molecular structure (Fig. 1), the Co^{II} atom is located on a crystallographic inversion center, and is in a slightly distorted octahedral CoN_2O_4 coordination geometry (Table 1).



In the crystal structure, intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{S}$ hydrogen bonds (Table 2) link the molecules into a three-dimensional network.

Experimental

An aqueous solution (5 ml) of 3-hydroxypyridine *N*-oxide (0.1556 g, 1.40 mmol) was added to an aqueous solution (15 ml) of $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.2617 g, 0.715 mmol) and NaNCS (0.1156 g, 1.43 mmol), and the mixture was stirred for a few minutes. Light-red single crystals were obtained after the solution was allowed to stand at room temperature for two weeks. The infrared spectrum reveals that there is a strong peak at 2110 cm^{-1} for the vibration of the thiocyanate ligand, and peaks at 1615 and 1592 cm^{-1} for the vibrations of pyridine ring.

Crystal data

$[\text{Co}(\text{NCS})_2(\text{C}_5\text{H}_5\text{NO}_2)_2(\text{H}_2\text{O})_2]$
 $M_r = 433.32$
Monoclinic, $P2_1/c$
 $a = 5.3123$ (10) Å
 $b = 14.199$ (3) Å
 $c = 12.063$ (2) Å
 $\beta = 97.347$ (2)°
 $V = 902.4$ (3) Å³

$Z = 2$
 $D_x = 1.595$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 1.22$ mm⁻¹
 $T = 298$ (2) K
Prism, red
 $0.45 \times 0.21 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.610$, $T_{\max} = 0.811$

4829 measured reflections
 1773 independent reflections
 1607 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.069$
 $S = 1.04$
 1773 reflections
 117 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.1913P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.007$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0067 (17)

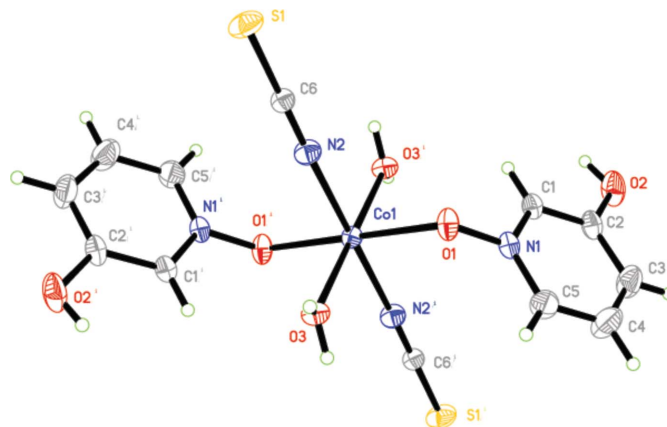


Figure 1
 The molecular structure of (I), showing the atom-numbering scheme with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, -y + 1, -z$].

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co1—O1	2.0675 (12)	Co1—O3	2.1148 (12)
Co1—N2	2.0829 (15)		
O1 ⁱ —Co1—O1	180	N2—Co1—O3	89.76 (5)
O1—Co1—N2 ⁱ	91.54 (6)	O1—Co1—O3 ⁱ	90.50 (5)
O1—Co1—N2	88.46 (6)	N2—Co1—O3 ⁱ	90.24 (5)
N2 ⁱ —Co1—N2	180	O3—Co1—O3 ⁱ	180
O1—Co1—O3	89.50 (5)		

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

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H6 \cdots O1 ⁱⁱ	0.84	1.85	2.6845 (18)	172
O3—H7 \cdots O2 ⁱⁱⁱ	0.84	2.01	2.8393 (19)	170
O2—H2 \cdots S1 ^{iv}	0.82	2.40	3.2025 (18)	165

Symmetry codes: (ii) $-x, -y + 1, -z$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x + 1, -y + \frac{3}{2}, z + \frac{1}{2}$.

The H atoms of the coordinated H_2O molecules were located in a difference Fourier, but were subsequently refined in a riding-model

approximation with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. All other H atoms were placed in calculated positions and refined in a riding-model approximation, with $\text{C—H} = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $\text{O—H} = 0.82 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ for the hydroxyl H atom.

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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