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Diaquadiisothiocyanatobis(pyridine *N*-oxide)-cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.124
Data-to-parameter ratio = 13.6

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

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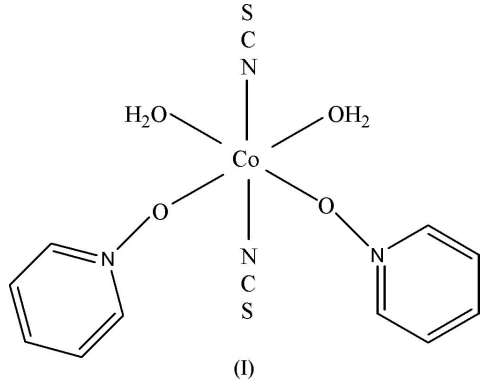
In the title mononuclear complex, $[Co(NCS)_2(C_5H_5NO)_2(H_2O)_2]$, cobalt(II) has a distorted octahedral coordination formed by two N atoms from two thiocyanate anions and four O atoms from two water molecules and two pyridine *N*-oxide molecules. The complexes are connected to each other by O—H···O and O—H···S hydrogen bonds.

Comment

Fig. 1 shows the title complex, (I), in which atom Co1 is coordinated by two N atoms from thiocyanate anions and four O atoms from two water molecules and two pyridine *N*-oxide molecules. As indicated in Fig. 1, atom Co1 has a distorted octahedral coordination. Various hydrogen bonds (Table 1 and Fig. 2) help to stabilize the crystal packing. The coordinated water molecule O2 forms two O—H···O bonds to *N*-oxide O-atom acceptors. The coordinated water molecule O1 forms O—H···O and O—H···S bonds, the acceptor O atom being the O atom of the pyridine *N*-oxide.



(I)

Experimental

Pyridine *N*-oxide (0.0639 g, 0.672 mmol) was added to an aqueous solution (12 ml) containing $Co(ClO_4)_2·6H_2O$ (0.1253 g, 0.342 mmol) and sodium thiocyanate (0.0562 g, 0.693 mmol), and the solution was stirred for a few minutes. Pink single crystals of (I) were obtained after the solution had been allowed to stand at room temperature for three weeks.

Crystal data

$[Co(NCS)_2(C_5H_5NO)_2(H_2O)_2]$
M_r = 401.32
Triclinic, $P\overline{1}$
a = 5.4773 (15) Å
b = 11.326 (3) Å
c = 13.726 (4) Å
α = 86.366 (4)°
β = 78.985 (4)°
γ = 88.921 (4)°
V = 834.1 (4) Å^3
Z = 2
D_x = 1.598 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1753 reflections
θ = 2.4–26.3°
μ = 1.30 mm^{-1}
T = 298 (2) K
Prism, pink
0.20 × 0.09 × 0.08 mm

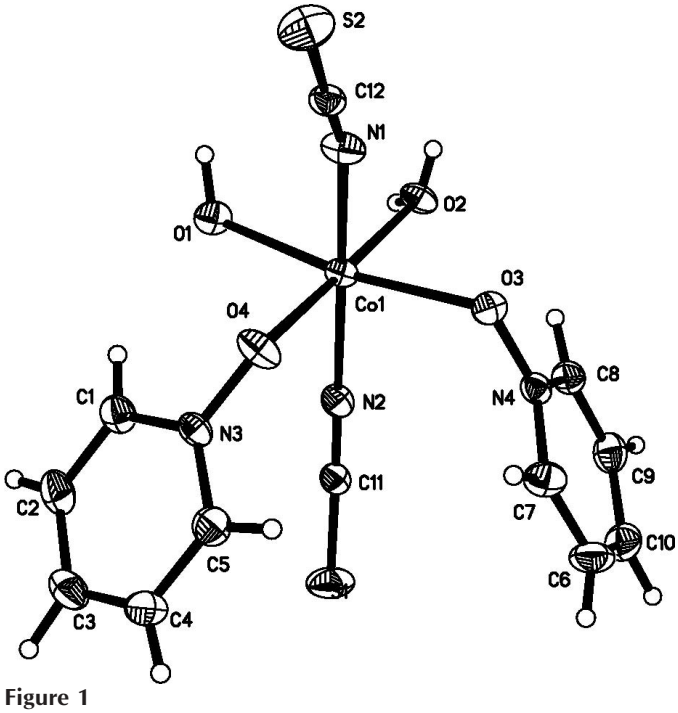


Figure 1
View of (I), showing 30% displacement ellipsoids. H atoms are shown as spheres of arbitrary radius.

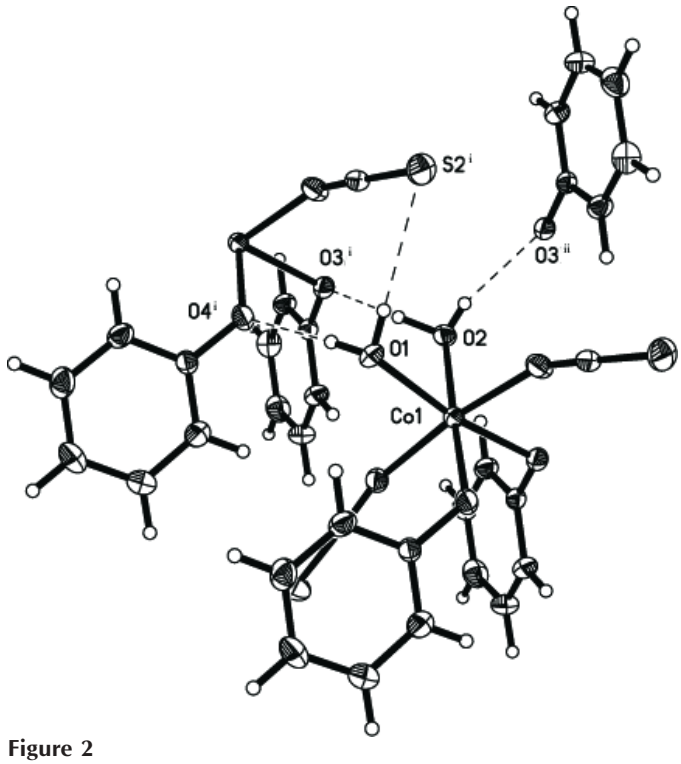


Figure 2
Hydrogen bonds (shown as broken lines) between the complex molecules. Symmetry codes are as in Table 1.

Data collection

Bruker SMART CCD area-detector diffractometer	2892 independent reflections
φ and ω scans	2582 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.022$
$T_{min} = 0.781$, $T_{max} = 0.903$	$\theta_{max} = 25.0^{\circ}$
4291 measured reflections	$h = -6 \rightarrow 6$
	$k = -11 \rightarrow 13$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 1.1096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.124$	$\Delta\rho_{max} = 0.35$ e Å^{-3}
$S = 1.14$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
2892 reflections	
212 parameters	
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···S2^{i}	0.87	2.59	3.433 (3)	164
O1—H12···O4^{i}	0.89	1.87	2.753 (4)	175
O2—H14···O3^{i}	0.99	1.86	2.833 (4)	165
O2—H13···O3^{ii}	0.71	2.23	2.901 (4)	157

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

H atoms bonded to C atoms were included in calculated positions. Other H atoms were located in a difference map. All H atoms were refined using a riding model [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C); O—H = 0.71–0.99 Å and U_{iso}(H) = 1.2U_{eq}(O)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 2001; software used to prepare material for publication: *SHELXTL*.

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