Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquadithiocyanatocobalt(II) bis(2-methylpyrazine 1,4-dioxide)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.083
Data-to-parameter ratio = 12.0

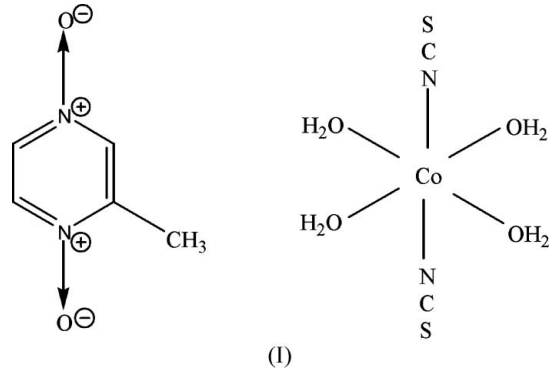
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 June 2005
Accepted 4 July 2005
Online 9 July 2005

In the crystal structure of the title compound, $[Co(NCS)_2(H_2O)_4]\cdot 2C_5H_6N_2O_2$, the six-coordinated Co^{II} complex lies on a special position of site symmetry 2/*m*. The methylpyrazine dioxide lies on a mirror plane and links with the Co^{II} complex *via* O—H···O hydrogen bonding.

Comment

The thiocyanate anion and pyrazine 1,4-dioxide are common bridging ligands for preparing polynuclear complexes (Shi *et al.*, 2005; Sun *et al.*, 2001). In order to understand the relationship between reaction conditions and the products, the title complex, (I), was synthesized and its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The Co^{II} atom lies on a special position of site symmetry 2/*m*. Four water O and two thiocyanate N atoms coordinate to the Co^{II} atom in an octahedral geometry (Table 1). The 2-methyl-

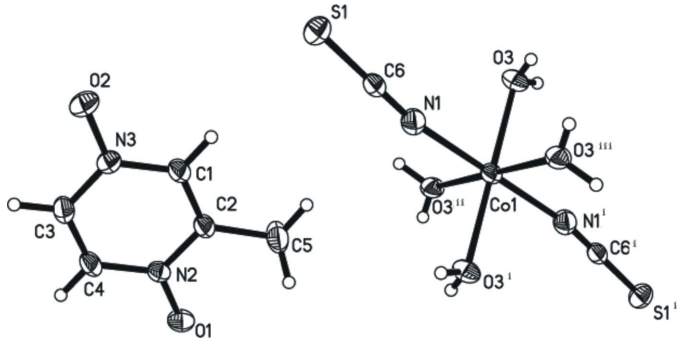


Figure 1
The molecular structure of (I) shown with 30% probability displacement ellipsoids (arbitary spheres for H atoms). [Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $-x+1, y, -z+2$; (iii) $x, -y, z$.]

pyrazine 1,4-dioxide, except for two methyl H atoms, lies on a mirror plane and links with the Co^{II} complex *via* O—H···O hydrogen bonding (Table 2). The structure is similar to the Mn^{II} analogue (Xu *et al.*, 2005).

Experimental

2-Methylpyrazine 1,4-dioxide (0.0436 g, 0.35 mmol) was added to an aqueous solution (15 ml) containing $Co(ClO_4)_2{\cdot}6H_2O$ (0.124 g, 0.34 mmol) and sodium thiocyanate (0.057 g, 0.70 mmol). The mixture was stirred for a few minutes and allowed to stand at room temperature. Pink single crystals of (I) were obtained after three weeks.

Crystal data

$[Co(NCS)_2(H_2O)_4]{\cdot}2C_5H_6N_2O_2$
M_r = 499.39
Monoclinic, $C2/m$
a = 16.982 (4) Å
b = 6.7616 (14) Å
c = 10.120 (2) Å
β = 111.718 (4)°
V = 1079.5 (4) Å^3
Z = 2
D_x = 1.536 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2566 reflections
θ = 2.6–28.1°
μ = 1.04 mm^{-1}
T = 298 (2) K
Prism, pink
0.20 × 0.16 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.815, T_{max} = 0.898
2873 measured reflections
1095 independent reflections
1045 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.5°
$h = -17 \rightarrow 20$
$k = -8 \rightarrow 8$
$l = -12 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.083
S = 1.12
1095 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.4739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.071 (4)

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.094 (2)	Co1—O3	2.1102 (12)
N1—Co1—O3	86.46 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H2···O1^{i}	0.85	1.94	2.746 (2)	159
O3—H1···O2^{ii}	0.86	1.87	2.7175 (19)	166

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

Pyrazine H atoms were placed in calculated positions. Other H atoms were located in a difference Fourier map. All H atoms were refined using a riding model, with C—H = 0.91–0.96 Å, O—H = 0.85–0.86 Å and U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank the Natural Science Foundation of China (No. 20271043) and the Natural Science Foundation of Shandong Province of China (No. Y2002B10) for support.

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