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Diaquabis(2-methylpyrazine-*N*)bis(thiocyanato-*N*)-cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.079
Data-to-parameter ratio = 22.8

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

In the structure of the title compound, $[Co(SCN)_2(C_5H_6N_2)_2(H_2O)_2]$, the cobalt cation is surrounded by two water molecules, two thiocyanate anions and two 2-methylpyrazine ligands in a slightly distorted octahedron. The cobalt cation is located on a centre of inversion and all other atoms are located in general positions. For the 2-methylpyrazine ligand, only the N atom which is not adjacent to the methyl group is involved in cobalt coordination. The complexes are connected *via* O—H···N and O—H···S hydrogen bonding, forming sheets parallel to (010).

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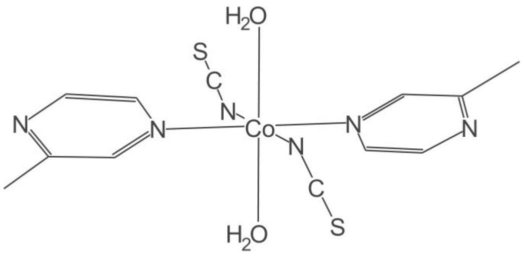
Comment

We have worked on the preparation, structural characterization and properties of new coordination polymers based on transition metal cations, aromatic amine ligands and pseudohalide anions. As ligands we used aromatic amines, which contain two N atoms in 1,4 positions, such as 2-methylpyrazine, which can act as bridging ligands *via* μ-*N*,*N*′ coordination, forming typical coordination polymers, *e.g.* *catena*-[bis(μ-2-methylpyrazine-*N*,*N*′)bis(μ-cyano-*C*,*N*)dicopper(I)], *catena*-[bis(μ-cyano-*C*,*N*)(μ-2-methylpyrazine-*N*,*N*′)dicopper(I)] and *catena*-[bis(μ-2-methylpyrazine-*N*,*N*)bis(μ-thiocyanato-*N*,*S*)dicopper(I)] (Teichert & Sheldrick, 1999) or poly[bis(μ-2-methylpyrazine)bis(cyanato)copper(II)] (Otieno *et al.*, 1993). Only a few structures are reported in the Cambridge Structural Database (Version 1.2, April 2001; Allen & Kennard, 1993) having a 2-methylpyrazine ligand, but none contain cobalt as the transition metal.



(I)

In the structure of the title compound, (I), the cobalt cation is located on a centre of inversion and all other atoms are located in general positions. The cobalt cation is sixfold coordinated by two O atoms of two water molecules, two N atoms of two 2-methylpyrazine ligands and two N atoms of the thiocyanato ligands. Bond lengths and angles are in the usual

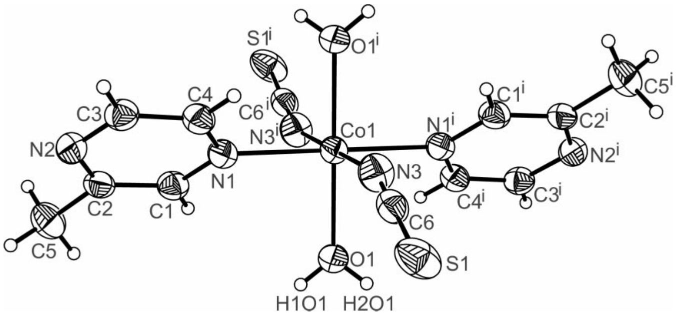


Figure 1

The structure of the title compound with a view of the cobalt coordination and atom labelling [displacement ellipsoids drawn at the 50% probability level; symmetry code: (i) $-x$, $-y$, $-z+1$].

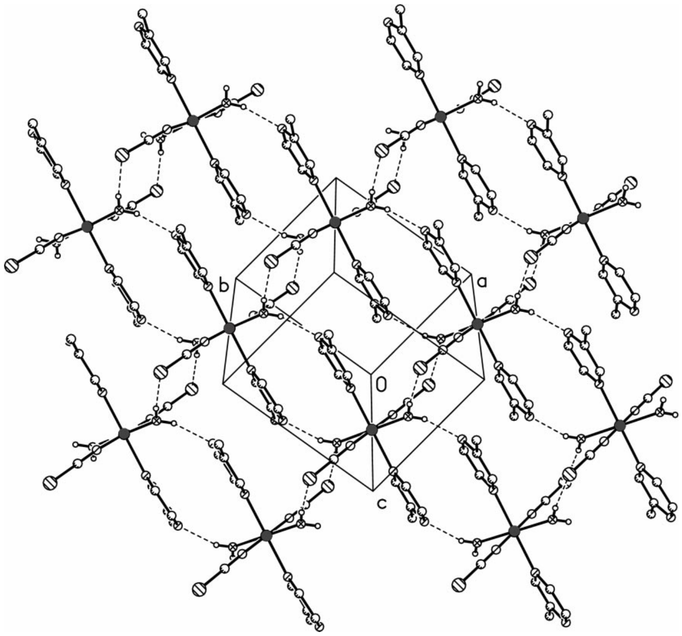


Figure 2

The crystal structure viewed along (010) showing the hydrogen-bonding pattern (hydrogen bonding is shown as dashed lines).

range compared with those of structures retrieved from the Cambridge Structural Database (Allen & Kennard, 1993) and the coordination polyhedron around the cobalt cation can be described as a slightly distorted octahedron. As expected, the Co—N bond lengths to the negatively charged thiocyanate anions are significantly shorter than those to the neutral ligands.

The 2-methylpyrazine molecules do not act as bridging ligands and only the N atom which is not adjacent to the methyl group is involved in cobalt coordination. This cannot be considered due only to sterically repulsion between the H atoms of the methyl group and the cobalt cation which would appear in the hexacoordinated complex, because in poly-[bis(μ-2-methylpyrazine)bis(cyanato)copper(II)] (Otieno *et al.*, 1993), in which the transition metal is also hexacoordinated and of approximately comparable size, the N atom which is the neighbour of the methyl group of the 2-methylpyrazine ligand is involved in the transition metal coordination. It is highly likely that in the title compound this is due to hydrogen bonding because the N atom adjacent to the methyl group acts as an acceptor for a H atom of a water molecule of a symmetry-related complex. The geometry of this interaction indicates strong hydrogen bonding, because two O—H···N hydrogen bonds between neighbouring complexes are formed; these are located around a centre of inversion, forming chains in the direction of the crystallographic *a* axis. The chains are connected further by short contacts between the S atoms of the thiocyanate anions and the H atoms of the water molecules, indicative of O—H···S hydrogen bonding. Two such contacts occur between neighbouring complexes located around centres of inversion. The O—H···N and O—H···S hydrogen bonding leads to sheets parallel to (010).

Experimental

The title compound was prepared by the reaction of 119.95 mg (0.5 mmol) $Co^{II}Cl_2\cdot 6H_2O$, 97.51 mg (1 mmol) KSCN and 0.094 ml (1 mmol) 2-methylpyrazine (ACROS) in 5 ml water at room temperature in a glass container. After three weeks, the residue was filtered off and washed with ethanol and diethyl ether. The precipitate is not pure and consists of yellow crystals of the title compound and a small amount of a microcrystalline powder, which could not be identified using X-ray powder diffraction.

Crystal data

$[Co(SCN)_2(C_5H_6N_2)_2(H_2O)_2]$
$M_r = 399.36$
Triclinic, $P\overline{1}$
$a = 6.910$ (2) Å
$b = 8.085$ (2) Å
$c = 9.234$ (2) Å
$\alpha = 107.85$ (1)°
$\beta = 111.93$ (1)°
$\gamma = 99.42$ (1)°
$V = 432.32$ (19) Å^3

$Z = 1$
$D_x = 1.534$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 92 reflections
$\theta = 11$–$17.5°$
$\mu = 1.25$ mm^{-1}
$T = 293$ (2) K
Block, yellow-orange
0.12 × 0.08 × 0.06 mm

Data collection

Stoe AED-II four-circle diffractometer
ω–θ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{min} = 0.796$, $T_{max} = 0.876$
2790 measured reflections
2513 independent reflections
1972 reflections with $I > 2\sigma(I)$

$R_{int} = 0.033$
$\theta_{max} = 30.0°$
$h = -9 \rightarrow 0$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$
4 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.06$
2513 reflections
110 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.0709P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.013 (3)

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Table 1
Selected geometric parameters (Å, °).

Co1—N3	2.0798 (17)	Co1—N1	2.1756 (15)
Co1—O1	2.0930 (14)		
$N3^{i}$—Co1—N3	180.0	O1—Co1—N1	91.33 (6)
$N3^{i}$—Co1—O1	91.55 (7)	$O1^{i}$—Co1—N1	88.67 (6)
N3—Co1—O1	88.45 (7)	N1—Co1—$N1^{i}$	180.0
O1—Co1—$O1^{i}$	180.0	C1—N1—Co1	121.70 (11)
$N3^{i}$—Co1—N1	88.77 (6)	C4—N1—Co1	121.41 (11)
N3—Co1—N1	91.23 (6)		

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

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1O1⋯$S1^{i}$	0.82	2.43	3.2508 (17)	173
O1—H2O1⋯$N2^{ii}$	0.82	2.03	2.816 (2)	160

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

The positions of all H atoms were located from a difference map. The C—H H atoms were positioned with idealized geometry and refined using a riding model. The positions of the methyl H atoms were idealized, then refined as rigid groups allowed to rotate but not tip. The H atoms of the water molecules were identified from difference syntheses and refined as rigid groups with idealized O—H bond lengths of 0.82 Å. Their isotropic displacement parameters were refined. All other H atoms were refined using fixed isotropic displacement parameters [$U_{\rm iso}$(H) = 1.5$U_{\rm eq}$C(methyl)].

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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