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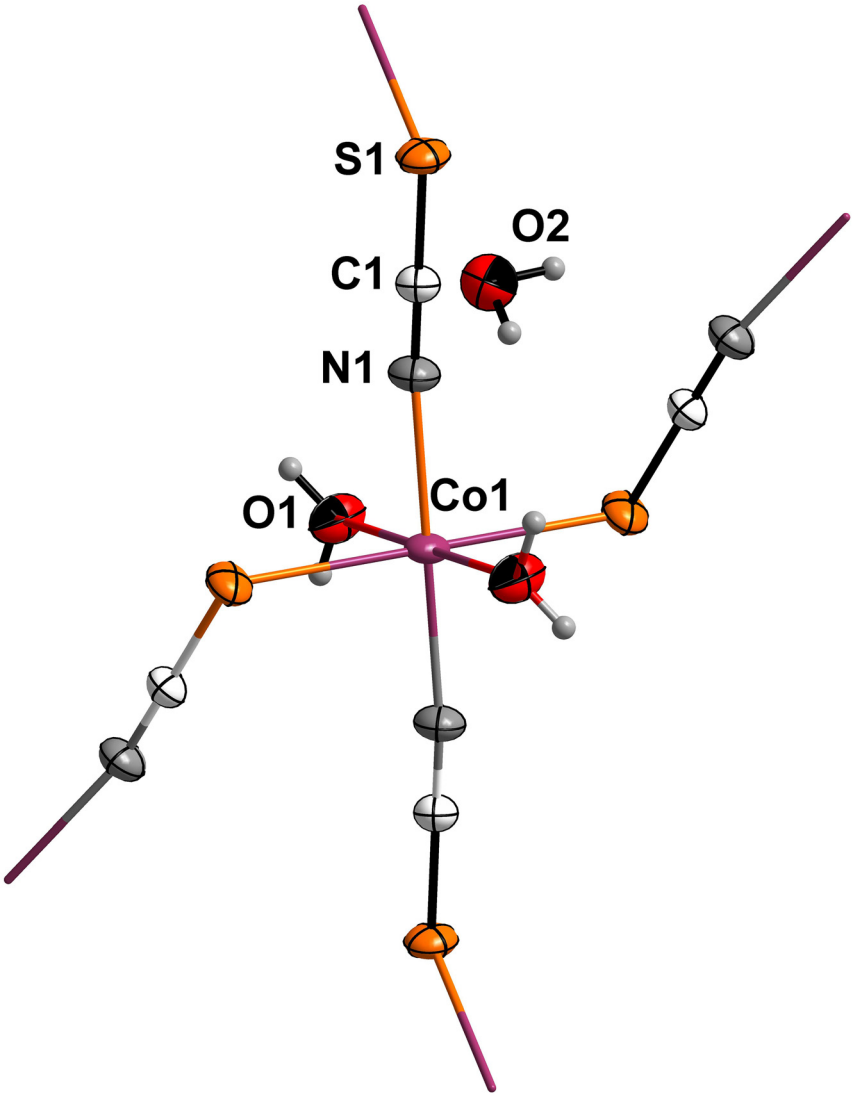
The crystal structure of poly[diaqua-bis(μ_2 -thiocyanato-κ^2*N:O*)cobalt(II) monohydrate



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Abstract

$C_2H_6S_2N_2O_3Co$, monoclinic, *C*2/*c* (no. 15), a = 12.4340(7) Å, b = 6.0522(4) Å, c = 10.6851(8) Å, β = 90.543(6)°, V = 804.05(9) Å^3, Z = 4, $R_{gt}(F)$ = 0.0200, $wR_{ref}(F^2)$ = 0.0499, T = 298(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of

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Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.12 × 0.10 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	2.61 mm^{-1}
Diffractometer, scan mode:	Dtrek-CrysAlis Pro-abstract goniometer, ω
θ_{max}, completeness:	32.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3,031, 1,378, 0.010
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1,287
$N(param)_{refined}$:	60
Programs:	SHELX,[1,2] Olex2[3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.250000	0.750000	0.500000	0.02224 (7)
S1	0.11068 (2)	0.51753 (4)	0.09801 (2)	0.02929 (8)
O1	0.37379 (7)	0.52136 (15)	0.52664 (9)	0.03571 (19)
O2	0.500000	0.5697 (3)	0.250000	0.0454 (3)
N1	0.20929 (7)	0.61882 (17)	0.32875 (8)	0.03063 (19)
C1	0.16954 (8)	0.57691 (16)	0.23367 (9)	0.02389 (18)
H2	0.539 (3)	0.657 (6)	0.215 (3)	0.144 (13)*
H1A	0.3699 (15)	0.405 (4)	0.4973 (19)	0.062 (6)*
H1B	0.4092 (16)	0.517 (3)	0.593 (2)	0.056 (5)*

the atoms including atomic coordinates and displacement parameters.

1 Source of materials

A mixture of $CoCl_2{\cdot}6H_2O$ (0.0476 g, 0.2 mmol), KSCN (0.0389 g, 0.4 mmol) and methanol (5 mL) was stirred for 30 min in air, sealed in a thick walled glass tube (10 mL) and then to evaporate at room temperature for 3 days.

2 Experimental details

Diffraction data were collected with a Rigaku XtaLAB single crystal diffractometer.[1,2] The structure was solved by Direct Methods and refined using the SHELXTL package. Hydrogen atoms were generated geometrically.[2,3]

3 Comment

As one of polydentate ligands, thiocyanate can be used to synthesize metal-thiocyanate complexes by virtue of the soft coordination site (S atom) or hard coordination site (N atom) with metal ions. Due to the strong super exchange interactions between paramagnetic metal centers, these materials are showing potential for magnetic applications.[4] Therefore, the assemble and application of metal-thiocyanate complexes have attracted great attention.[5–7] The title structure crystallizes in the monoclinic space group *C*2/*c*, containing one SCN^-, one coordinated H_2O and 0.5 Co^{2+} ion, as well as $0.5H_2O$ guest molecule in an asymmetric unit. Specifically, Co1 is six-coordinated with four SCN^- and two coordinated H_2O molecules. The adjacent Co^{2+} ions are bridged by SCN^- to construct a two-dimensional layer. These 2D layers are further connected with H_2O molecules in hydrogen bonds to obtain a three-dimensional network. All parameters are in the expected ranges.[8,9]

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Competing interests: The authors declare no conflicts of interest regarding this article.

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