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Crystal structures of two $Co(NCS)_2$ urotropine coordination compounds with different Co coordinations

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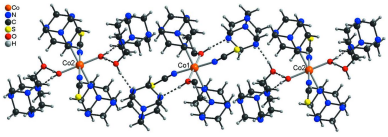
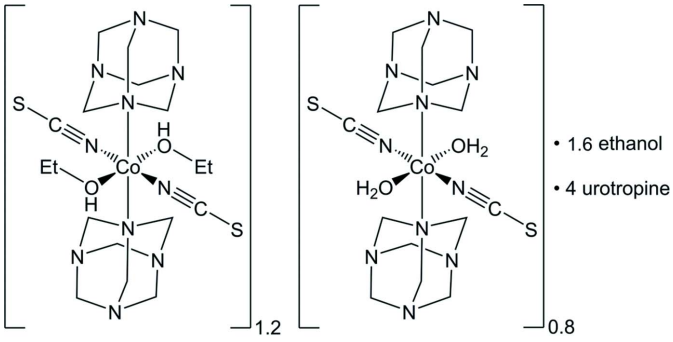
The reaction of $Co(NCS)_2$ with urotropine in ethanol leads to the formation of two different compounds, namely, bis(ethanol-κO)bis(hexamethylenetetramine-κN)bis(thiocyanato-κN)cobalt(II)–diaqua-$\kappa^2 O$-bis(hexamethylenetetramine-κN)bis(thiocyanato-κN)cobalt(II)–ethanol–hexamethylenetetramine (1.2/0.8/1.6/4), $[Co(NCS)_2(C_6H_{12}N_4)_2(C_2H_6O)_2]_{1.2}\cdot[Co(NCS)_2(C_6H_{12}N_4)_2(H_2O)_2]_{0.8}\cdot 1.6C_2H_6O\cdot 4C_6H_{12}N_4$, **1**, and tris(ethanol-κO)(hexamethylenetetramine-κN)bis(thiocyanato-κN)cobalt(II), $[Co(NCS)_2(C_6H_{12}N_4)(C_2H_6O)_3]$, **2**. In the crystal structure of compound **1**, two crystallographically independent discrete complexes are observed that are located on centres of inversion. In one of them, the Co cation is octahedrally coordinated to two terminal N-bonded thiocyanate anions, two urotropine ligands and two ethanol molecules, whereas in the second complex 80% of the coordinating ethanol is exchanged by water. Formally, compound **1** is a mixture of two different complexes, *i.e.* diaqua-dithiocyanatobis(urotropine)cobalt(II) and diethanoldithiocyanatobis(urotropine)cobalt(II), that contain additional ethanol and urotropine solvate molecules leading to an overall composition of $[Co(NCS)_2(urotropine)_2(ethanol)_{1.2}(H_2O)_{0.8}\cdot 0.8ethanol\cdot 4urotropine$. Both discrete complexes are linked by intermolecular O—H···O and O—H···N hydrogen bonding and additional urotropine solvate molecules into chains, which are further connected into layers. These layers combine into a three-dimensional network by pairs of centrosymmetric intermolecular C—H···S hydrogen bonds. In the crystal structure of compound **2**, dithiocyanato(urotropine)triethanolcobalt(II), the cobalt cation is octahedrally coordinated to two terminal N-bonded thiocyanate anions, one urotropine ligand and three ethanol molecules into discrete complexes, which are located in general positions. These complexes are linked by intermolecular O—H···N hydrogen bonding into layers, which are further connected into a three-dimensional network by intermolecular C—H···S hydrogen bonding.



1. Chemical context

Recently, we reported the crystal structure of two new coordination compounds with the composition $[Co(NCS)_2(urotropine)_2(ethanol)_2]$ and $[Co(NCS)_2(ethanol)_4](urotropine)_2$ (Krebs *et al.*, 2022). Both compounds consist of discrete complexes, in which the cobalt cations are octahedrally coordinated by two terminal N-bonded thiocyanate anions and by four ethanol and two ethanol and two urotropine ligands, respectively. These investigations were performed to prepare precursors that on thermal decomposition transform into coordination polymers in which the cobalt cations are linked by μ-1,3 bridging thiocyanate anions into chains or layers (Näther *et al.*, 2013). Several such compounds have been

reported in the literature and they are of interest because they show ferromagnetic or antiferromagnetic ordering or a slow relaxation of the magnetization, which is indicative for single-chain magnetism (Böhme *et al.*, 2020; Shi *et al.*, 2006; Jin *et al.*, 2007; Jochim *et al.*, 2020; Prananto *et al.*, 2017; Mautner *et al.*, 2018; Rams *et al.*, 2020; Ceglarska *et al.*, 2021; Werner *et al.*, 2014, 2015; Suckert *et al.*, 2016; Wellm *et al.*, 2020). In this context, urotropine as a coligand was of interest because this ligand is able to form networks (Czubacka *et al.*, 2012; Li *et al.*, 2012), is magnetically silent and one compound with cadmium had already been reported in which the metal cations are linked by the anionic ligands into chains (Bai *et al.*, 2009).



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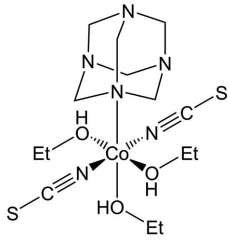

2

However, for the preparation of the two compounds mentioned above, cobalt thiocyanate was reacted with urotropine in ethanol and X-ray powder measurements show that none of these compounds can be prepared as a pure crystalline phase. Either the desired compounds were obtained as the minor phase or the experimental powder patterns were completely different from the calculated one. These investigations indicate that additional compounds are present and that the desired compounds are not very stable and transform in solution. Therefore, additional crystallization experiments were performed, which lead to the formation of single crystals of two new compounds that were identified by single crystal X-ray diffraction. Even these compounds contain ethanol as a ligand but in one compound one coordination site is simultaneously occupied by ethanol and water, which might originate from some residual water in the solvent used in the synthesis, whereas in the second compound the cobalt cations are coordinated by only one urotropine and three ethanol ligands. All this indicates that, for this system, different species are in equilibrium in solution and some phase crystallizes, presumably by kinetic control, which means that the synthesis is difficult to control.

2. Structural commentary

The asymmetric unit of compound **1** consists of two crystallographically independent Co cations that are located on centres of inversion as well as two thiocyanate anions, four urotropine ligands, three ethanol and one water molecule that occupy general positions (Fig. 1). One of the cobalt cations (Co1) is sixfold coordinated to two terminal N-bonded thiocyanate anions, two urotropine ligands and two ethanol molecules into discrete complexes (Fig. 1, top left). The methyl carbon atom of these ethanol molecules is disordered in two positions and was refined using a split model. The second cobalt cation is also sixfold coordinated, forming discrete complexes, to two terminal N-bonded thiocyanate anions, two urotropine ligands and two oxygen atoms, but the latter positions are mixed occupied by water and ethanol in a ratio of 8:2, leading to an overall composition for **1** of $[Co(NCS)_2(urotropine)_2(ethanol)_{1.2}(H_2O)_{0.8}\cdot 1.6ethanol\cdot\cdot 4urotropine$. In the case where it is occupied by water, an ethanol molecule is hydrogen bonded to this water molecule; if it is occupied by ethanol, this ethanol solvate molecule is not present (Fig. 1, top right). The position of the disordered O atoms of the water and ethanol molecule was resolved and all O—H H atoms were clearly located in the difference map and refined isotropically with reasonable displacement parameters, using restraints for the O—H distances (see *Refinement*). The Co—N bond lengths to the thiocanate anions are similar in both complexes, which is also valid for the bond length to the urotropine ligands (Table 1). In contrast, the Co—O bond length to the water molecule is shorter than

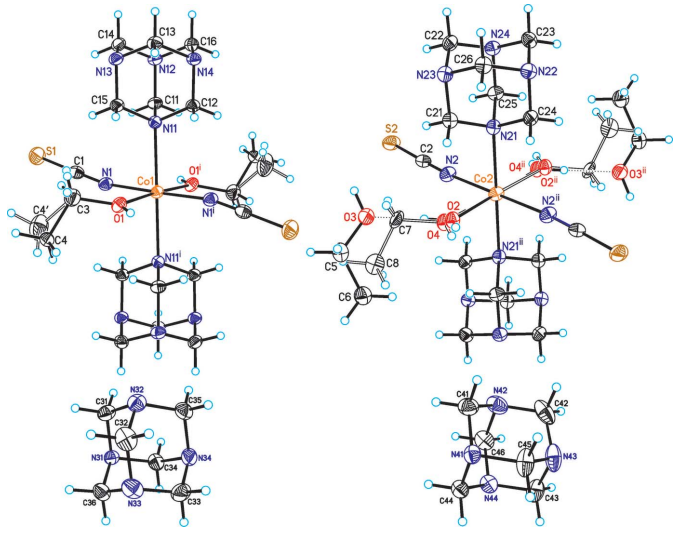

Figure 1
Crystal structure of compound **1** with labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code for the generation of equivalent atoms: (i) $-x+1, -y+1, -z+2$; (ii) $-x+2, -y+1, -z+1$.

Table 1
Selected bond lengths (Å) for **1**.

Co1—N1	2.0590 (16)	Co2—O2	2.029 (6)
Co1—O1	2.1388 (13)	Co2—O4	2.21 (3)
Co1—N11	2.2834 (15)	Co2—N21	2.2788 (16)
Co2—N2	2.0812 (16)		

Table 2
Selected bond lengths (Å) for **2**.

Co1—N2	2.0615 (11)	Co1—O31	2.1157 (9)
Co1—N1	2.0624 (11)	Co1—O21	2.1314 (9)
Co1—O41	2.1021 (10)	Co1—N11	2.2489 (11)

those to the ethanol molecules (Table 1), even if there might be some uncertainty in the distances because of the disorder.

The asymmetric unit of compound **2** consists of one crystallographically independent cobalt cation, one urotropine ligand and three ethanol molecules, all of them located in general positions (Fig. 2). In this compound the cobalt cations are sixfold coordinated to two terminal N-bonded thiocyanate anions, one urotropine ligand and three ethanol molecules. The Co—N and Co—O bond lengths are comparable to those in compound **1** and to similar ethanol complexes retrieved from the literature (Krebs *et al.*, 2021*a*, Table 2). From the angles around the Co cations, it is obvious that in all compounds the octahedra are slightly distorted (see supporting information). It is noted that compound **2** completes the series of $Co(NCS)_2$-urotropine compounds with ethanol as an additional ligand, because in this compound the cobalt cations are coordinated to one urotropine and three ethanol ligands, whereas in the other compounds reported recently the cobalt cations are either coordinated to two urotropine and two ethanol ligands or to four ethanol ligands (Krebs *et al.*, 2021*a*).

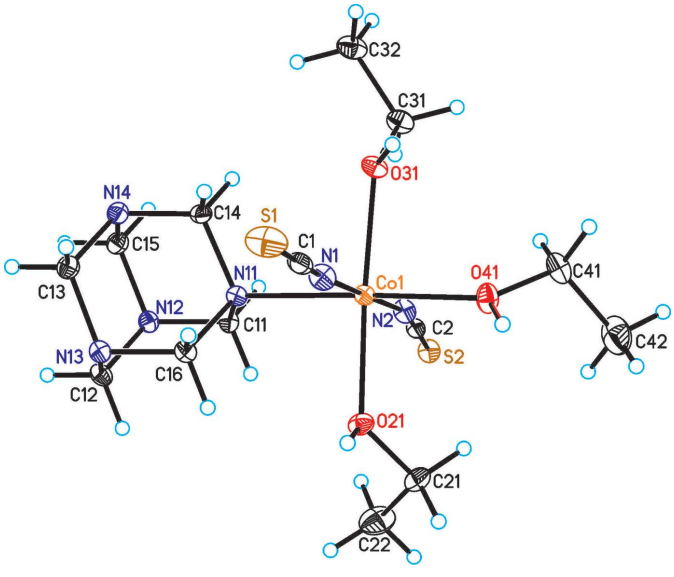

Figure 2
Crystal structure of compound **2** with labelling and displacement ellipsoids drawn at the 50% probability level.

Table 3
Hydrogen-bond geometry (Å, °) for **1**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N31	0.88 (2)	1.92 (2)	2.793 (2)	170 (3)
C4′—H4′*A*···N43^{i}	0.96	2.50	3.243 (14)	134
C4′—H4′*C*···N44^{ii}	0.96	2.38	3.161 (10)	138
O2—H2*A*···N41	0.87 (2)	1.88 (2)	2.743 (7)	173 (7)
O2—H2*B*···O3	0.87 (2)	1.80 (2)	2.665 (4)	177 (5)
C5—H5*A*···S2^{iii}	0.97	3.02	3.925 (3)	156
O3—H3···N34	0.87 (2)	1.97 (2)	2.821 (3)	167 (4)
O4—H4···N41	0.87 (2)	1.94 (5)	2.81 (3)	170 (19)
C11—H11*A*···O1^{ii}	0.97	2.49	3.058 (2)	117
C11—H11*B*···N1	0.97	2.67	3.213 (2)	116
C12—H12*B*···N44	0.97	2.64	3.423 (3)	138
C13—H13*A*···N13^{iv}	0.97	2.70	3.563 (2)	149
C13—H13*B*···S2^{iii}	0.97	2.95	3.7150 (19)	136
C14—H14*A*···S2^{v}	0.97	2.93	3.840 (2)	156
C15—H15*B*···O1	0.97	2.61	3.118 (2)	113
C22—H22*B*···N12^{vi}	0.97	2.58	3.448 (2)	149
C25—H25*A*···O2^{vii}	0.97	2.50	3.026 (7)	114
C25—H25*A*···O4^{vii}	0.97	2.49	3.08 (3)	119
C25—H25*B*···N2	0.97	2.61	3.202 (3)	119
C26—H26*A*···S1^{ii}	0.97	2.98	3.655 (2)	128
C26—H26*B*···N22^{viii}	0.97	2.69	3.581 (3)	152
C33—H33*A*···N23	0.97	2.66	3.431 (3)	137
C45—H45*A*···S2^{vii}	0.97	3.01	3.959 (3)	165

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y, -z+2$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+1$; (v) $x, y-1, z$; (vi) $x, y+1, z$; (vii) $-x+2, -y+1, -z+1$; (viii) $-x+2, -y+1, -z+2$.

3. Supramolecular features

In the crystal structure of the title compound, extensive hydrogen bonding is observed (Table 3). The discrete complex around Co1 is linked to two urotropine solvate molecules *via* intermolecular O—H···N hydrogen bonding (Fig. 3 and Table 3). For the Co2 complex, two different surroundings are observed. In the case where this cation is coordinated to water, this water molecule is hydrogen bonded to two urotropine ligands and two ethanol molecules (Fig. 4, top and Table 3). There are two additional C—H···S hydrogen bonds, which are not shown for clarity. In the case where Co2 is coordinated to

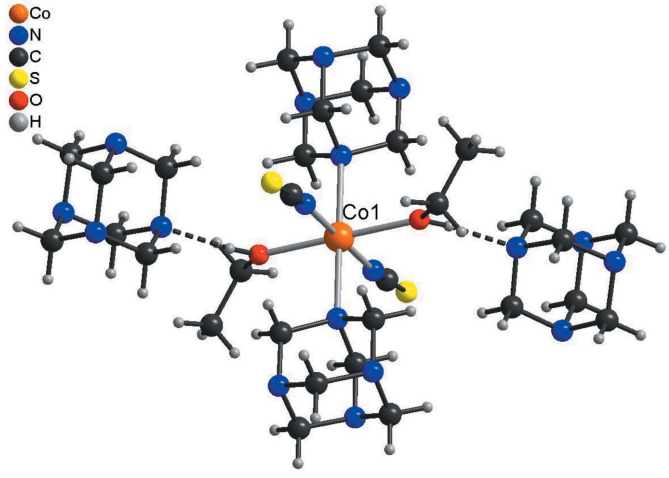

Figure 3
View of the discrete complex in compound **1** built up of Co1, which is connected to two urotropine solvate molecules *via* intermolecular O—H···N hydrogen bonding (shown as dashed lines).

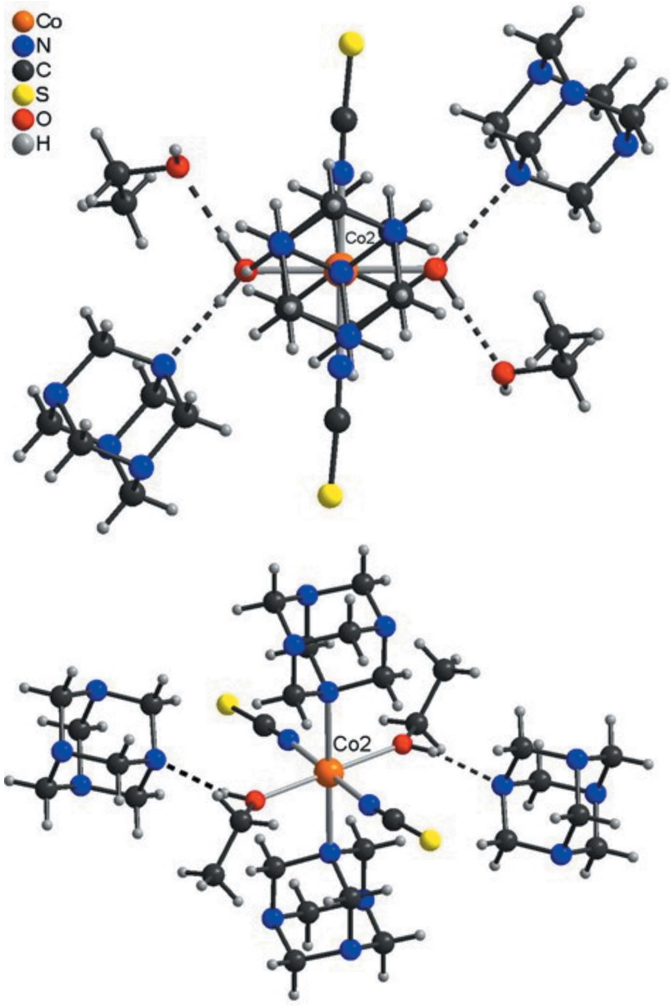

Figure 4
View of the two different coordinations of Co2 in compound **1** with H_2O (top) and ethanol (bottom) with intermolecular hydrogen bonding shown as dashed lines.

EtOH, the solvate ethanol molecule is not present and the surrounding is similar to that around Co1 with only hydrogen bonding to two urotropine ligands (compare Fig. 3 and Fig. 4, bottom). Both crystallographically independent complexes are linked into chains *via* intermolecular O—H···O and O—H···N hydrogen bonding (Fig. 5). The chains are further connected into layers by intermolecular C—H···O and C—H···N interactions. These layers are stacked onto each other

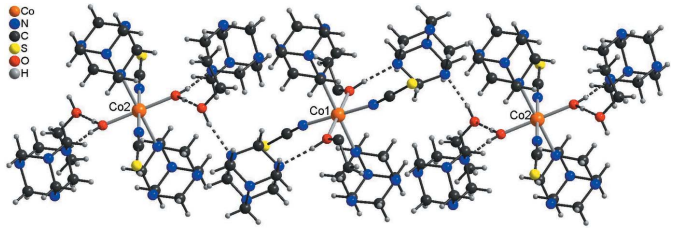

Figure 5
Part of the crystal structure of compound **1** showing the connection of the discrete complexes by the urotropine solvate molecules *via* intermolecular O—H···N hydrogen bonding (shown as dashed lines).

Table 4
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···S2^{i}	0.99	2.87	3.6586 (13)	137
C12—H12B···S1^{ii}	0.99	2.92	3.8813 (13)	164
C15—H15A···S1^{iii}	0.99	2.99	3.9387 (13)	161
C15—H15B···S2^{iv}	0.99	2.94	3.7110 (13)	135
C16—H16A···O21	0.99	2.54	3.1009 (16)	116
C16—H16B···N1	0.99	2.47	3.1083 (17)	122
O21—H21···N13^{ii}	0.84	2.03	2.8424 (14)	161
C22—H22C···S1^{v}	0.98	3.02	3.9559 (16)	161
O31—H31···N12^{vi}	0.84	1.96	2.7969 (14)	172
O41—H41···S2^{vi}	0.84	2.37	3.2080 (10)	174

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

and are linked by intermolecular centrosymmetric pairs of C—H···S hydrogen bonds, in which only the discrete complex built up of Co2 is involved (Fig. 6 and Table 3).

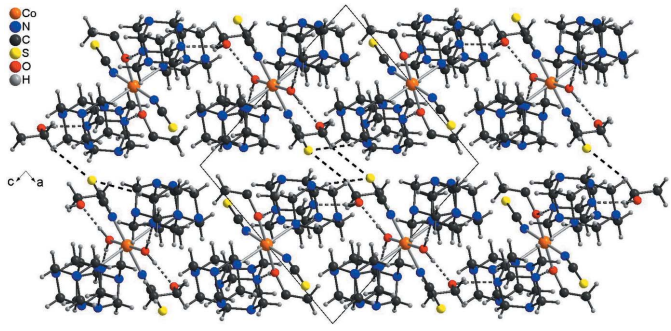

Figure 6
Crystal structure of compound **1** with a view along the crystallographic *b* axis and intermolecular hydrogen bonding shown as dashed lines.

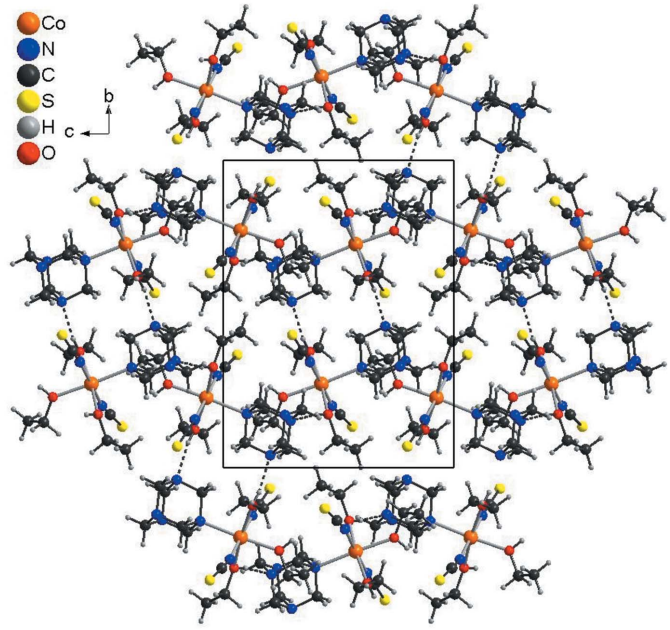

Figure 7
Crystal structure of compound **2** with a view along the crystallographic *a* axis and intermolecular O—H···N hydrogen bonding shown as dashed lines.

Table 5
Experimental details.

	1	2
Crystal data		
Chemical formula	$[Co(NCS)_2(C_6H_{12}N_4)_2(C_2H_6O)_2]_{1.2}\cdot[Co(NCS)_2(C_6H_{12}N_4)_2(H_2O)_2]_{0.8}\cdot 1.6C_2H_6O\cdot 4C_6H_{12}N_4$	$[Co(NCS)_2(C_6H_{12}N_4)(C_2H_6O)_3]$
M_r	1684.84	453.49
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	100	100
a, b, c (Å)	12.1536 (2), 12.9256 (3), 12.9374 (3)	11.1463 (1), 15.7705 (1), 12.1824 (1)
α, β, γ (°)	76.629 (2), 80.395 (2), 80.578 (2)	90, 103.886 (1), 90
V (Å^3)	1932.91 (7)	2078.87 (3)
Z	1	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	4.97	8.58
Crystal size (mm)	0.16 × 0.12 × 0.08	0.2 × 0.18 × 0.03
Data collection		
Diffractometer	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.693, 1.000	0.427, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25821, 8226, 7777	29441, 4431, 4373
R_{int}	0.024	0.027
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.639	0.635
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.103, 1.09	0.025, 0.068, 1.08
No. of reflections	8226	4431
No. of parameters	545	242
No. of restraints	10	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.82, −0.69	0.32, −0.31

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2014/4* and *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 1999), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

In the crystal structure of compound **2**, the discrete complexes are linked by strong intermolecular O—H···N hydrogen bonding between two of the three O—H hydrogen atoms of the ethanol ligands and two urotropine N atoms into layers that are parallel to the *bc* plane (Fig. 7 and Table 4). These layers are further linked by intermolecular O—H···S and C—H···S hydrogen bonding into a three-dimensional network (Table 4). Some of the O—H···S and C—H···S angles are close to linearity, indicating that these are relatively strong interactions (Table 4).

4. Database survey

In the Cambridge Structure Database (CSD version 5.42, last update November 2020; Groom *et al.*, 2016) there are already several structures reported that contain cobalt thiocyanate and urotropine as a ligand, but only one of them contains additional ethanol (Krebs *et al.*, 2021*a*). Most of them contain water as a ligand or solvate molecule. In $[Co(NCS)_2(H_2O)_4]\cdot 2$urotropine (Refcode: XILXOG; Li *et al.*, 2007), the cobalt cations are octahedrally coordinated by two thiocyanate anions and four water ligands with two additional urotropine ligands acting as solvate molecules. $[Co(NCS)_2(urotropine)_2(H_2O)_2][Co(NCS)_2(H_2O)_4]\cdot 2H_2O$ (Refcode: MOTNIS; Liu *et al.*, 2002, MOTNIS01; Zhang *et al.*, 1999, MOTNIS02; Chakraborty *et al.*, 2006, MOTNIS03; Lu *et al.*, 2010) consists of two crystallographically independent discrete complexes in which the cobalt cations are coordinated by two terminal N-bonded thiocyanate anions and four water or two water and two urotropine ligands with additional water as solvate molecules. There is also one complex with water and methanol as ligands with the composition $[Co(NCS)_2(urotropine)(CH_3OH)_2(H_2O)]$ (Refcode: POFGAT; Shang *et al.*, 2008), in which the cobalt cations are octahedrally coordinated by the N atoms of two thiocyanate anions, two methanol, one water and one urotropine ligand. Moreover, a compound with the composition $[Co(NCS)_2(urotropine)_2(CH_3CN)_2]$ that also consists of discrete complexes has been reported (Krebs *et al.*, 2021). It is noted that even with other metal cations only discrete complexes are reported, such as, for example, with nickel (Refcode: XILROA; Bai *et al.*, 2007, XILROA01; Lu *et al.*, 2010), or zinc (Refcode: SIMXIY; Kruszynski *et al.*, 2018). Finally, a crystal structure is reported with cadmium in which the Cd cations are linked by pairs of thiocyanate anions into chains, which are further linked by the urotropine ligand (Refcode: DOZZOI; Bai *et al.*, 2009).

5. Synthesis and crystallization

Synthesis $Co(NCS)_2$ and urotropine were purchased from Merck. All chemicals were used without further purification.

Crystals of compound **1** suitable for single-crystal X-ray diffraction were obtained after one day by the reaction of 0.15 mmol of $Co(NCS)_2$ (26.3 mg) with 0.60 mmol of urotropine (84.1 mg) in 1.0 mL of ethanol at room temperature. The reaction of 0.15 mmol of $Co(NCS)_2$ (26.3 mg) with 0.15 mmol of urotropine (21.0 mg) in 2.0 mL of ethanol at room temperature led to the formation of single crystals of compound **2**.

The data collection for single-crystal structure analysis was performed using an XtaLAB Synergy, Dualflex, HyPix diffractometer from Rigaku with Cu $K\alpha$ radiation.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. All non-hydrogen atoms were refined anisotropically. The C—H hydrogen atoms were located in the difference map but positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropically with $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5 for methyl H atoms) using a riding model. The O—H hydrogen atoms were located in the difference map and were refined with restraints for the O—H distance (DFIX) and varying isotropic displacement parameters in compound **1**, whereas in compound **2** they were positioned with idealized geometry allowed to rotate but not to tip and were refined isotropically with $U_{iso}(H) = 1.5U_{eq}(O)$ using a riding model. In compound **1**, the methyl group of the EtOH molecule coordinated to Co1 is disordered and was refined using a split model. In this compound, Co2 is either coordinated to water or to EtOH. In this case the O atoms occupy nearly the same crystallographic positions but finally both O atoms can be refined separately with anisotropic displacement parameters. In the case where Co2 is coordinated to water, it is hydrogen bonded to one EtOH solvate molecule. If Co2 is coordinated to EtOH, the position of the EtOH solvate molecule cannot be occupied. Therefore, the site occupation factor (sof) of the EtOH solvate molecule must be identical to that of the coordinated water molecule. In the beginning the sof was refined, leading to values close to 0.8 for the water and 0.2 for the coordinated EtOH molecule but in the final refinements it was fixed at 0.8 and 0.2. The H-atom positions of both, water and EtOH, were clearly located and were refined with restraints and varying isotropic displacement parameters. This leads to comparable and reasonable values for the O—H distances as well as for the isotropic displacement parameters of the O—H hydrogen atoms.

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supporting information

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Crystal structures of two $Co(NCS)_2$ urotropine coordination compounds with different Co coordinations

Christoph Krebs, Inke Jess and Christian Näther

Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021). Program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a) for (1); *SHELXT2014/4* (Sheldrick, 2015a) for (2). For both structures, program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b). Molecular graphics: *DIAMOND* (Brandenburg & Putz, 1999) for (1); *OLEX2* (Dolomanov *et al.*, 2009) for (2). Software used to prepare material for publication: *publCIF* (Westrip, 2010) for (1); *OLEX2* (Dolomanov *et al.*, 2009) for (2).

Bis(ethanol-*κO*)bis(hexamethylenetetramine-*κN*)bis(thiocyanato-*κN*)cobalt(II)–diaqua-*κ*^{2}*O*-bis(hexamethylenetetramine-*κN*)bis(thiocyanato-*κN*)cobalt(II)–ethanol–hexamethylenetetramine (1.2/0.8/1.6/4) (1)

Crystal data

$[Co(NCS)_2(C_6H_{12}N_4)_2(C_2H_6O)_2]_{1.2}\cdot[Co(NCS)_2(C_6H_{12}N_4)_2(H_2O)_2]_{0.8}\cdot 1.6C_2H_6O\cdot 4C_6H_{12}N_4$
M_r = 1684.84
Triclinic, $P\overline{1}$
a = 12.1536 (2) Å
b = 12.9256 (3) Å
c = 12.9374 (3) Å
α = 76.629 (2)°
β = 80.395 (2)°
γ = 80.578 (2)°
V = 1932.91 (7) Å^3
Z = 1
$F(000)$ = 898
D_x = 1.447 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 18138 reflections
θ = 3.7–79.3°
μ = 4.97 mm^{-1}
T = 100 K
Plate, light colourless
0.16 × 0.12 × 0.08 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.693, T_{max} = 1.000
25821 measured reflections
8226 independent reflections
7777 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 80.1°, θ_{min} = 3.5°
h = −15→15
k = −16→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.103
S = 1.09
8226 reflections
545 parameters
10 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 1.7899P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Extinction correction: SHELXL2016/6 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00080 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.500000	0.000000	1.000000	0.01667 (10)	
Co2	1.000000	0.500000	0.500000	0.01929 (11)	
N1	0.38177 (14)	−0.10448 (13)	1.03166 (13)	0.0209 (3)	
C1	0.31474 (16)	−0.15722 (15)	1.02515 (15)	0.0219 (4)	
S1	0.22329 (5)	−0.23250 (5)	1.01546 (5)	0.03988 (15)	
N2	0.85107 (14)	0.59836 (13)	0.46671 (13)	0.0238 (3)	
C2	0.76974 (17)	0.65684 (15)	0.45319 (15)	0.0226 (4)	
S2	0.65758 (5)	0.74450 (5)	0.43091 (5)	0.03506 (14)	
O1	0.37719 (11)	0.13161 (11)	0.94616 (11)	0.0216 (3)	
H1	0.392 (3)	0.1982 (16)	0.927 (3)	0.060 (10)*	
C3	0.26483 (18)	0.13151 (18)	0.91942 (18)	0.0294 (4)	
H3AA	0.250342	0.057923	0.930034	0.044*	0.8
H3AB	0.262932	0.164417	0.844216	0.044*	0.8
H3BC	0.250431	0.196444	0.865692	0.044*	0.2
H3BD	0.271029	0.072225	0.883622	0.044*	0.2
C4	0.1725 (2)	0.1909 (2)	0.98618 (19)	0.0200 (4)	0.8
H4A	0.100686	0.185071	0.968034	0.030*	0.8
H4B	0.183149	0.265097	0.971950	0.030*	0.8
H4C	0.175324	0.160103	1.060858	0.030*	0.8

C4′	0.1630 (6)	0.1249 (14)	0.9957 (8)	0.047 (3)	0.2
H4′A	0.104113	0.109715	0.962611	0.071*	0.2
H4′B	0.140682	0.191965	1.018112	0.071*	0.2
H4′C	0.176793	0.068708	1.056935	0.071*	0.2
O2	0.9172 (3)	0.3693 (6)	0.5467 (6)	0.0215 (6)	0.8
H2A	0.939 (5)	0.308 (3)	0.588 (5)	0.07 (3)*	0.8
H2B	0.8447 (17)	0.372 (4)	0.548 (4)	0.077 (18)*	0.8
O3	0.69673 (15)	0.37997 (14)	0.54414 (15)	0.0275 (4)	0.8
C5	0.6645 (2)	0.2810 (2)	0.5350 (2)	0.0267 (5)	0.8
H5A	0.586260	0.291950	0.523215	0.032*	0.8
H5B	0.672275	0.228069	0.600949	0.032*	0.8
C6	0.7380 (2)	0.2411 (2)	0.4427 (2)	0.0298 (5)	0.8
H6A	0.731836	0.294723	0.378049	0.045*	0.8
H6B	0.714164	0.176471	0.434837	0.045*	0.8
H6C	0.814805	0.226809	0.456517	0.045*	0.8
H3	0.656 (3)	0.406 (3)	0.597 (2)	0.054 (11)*	0.8
O4	0.8970 (16)	0.367 (3)	0.543 (3)	0.0215 (6)	0.2
C7	0.7799 (8)	0.3562 (8)	0.5603 (9)	0.026 (2)	0.2
H7A	0.736856	0.426993	0.546472	0.032*	0.2
H7B	0.759133	0.323060	0.634838	0.032*	0.2
C8	0.7500 (9)	0.2899 (8)	0.4899 (8)	0.030 (2)	0.2
H8A	0.762768	0.326382	0.416213	0.046*	0.2
H8B	0.672194	0.279629	0.508926	0.046*	0.2
H8C	0.796095	0.221486	0.499688	0.046*	0.2
H4	0.930 (14)	0.306 (9)	0.574 (17)	0.02 (5)*	0.2
N11	0.53970 (13)	−0.04050 (12)	0.83394 (12)	0.0169 (3)	
N12	0.59878 (13)	−0.18558 (13)	0.73316 (12)	0.0199 (3)	
N13	0.46941 (13)	−0.02933 (13)	0.66262 (12)	0.0201 (3)	
N14	0.66683 (13)	−0.01109 (12)	0.66326 (12)	0.0189 (3)	
C11	0.57045 (16)	−0.15859 (14)	0.83915 (14)	0.0193 (4)	
H11A	0.634285	−0.184309	0.878516	0.023*	
H11B	0.507809	−0.195364	0.878363	0.023*	
C12	0.63690 (15)	0.01248 (15)	0.77084 (14)	0.0189 (4)	
H12A	0.618761	0.089443	0.764292	0.023*	
H12B	0.701533	−0.011012	0.809414	0.023*	
C13	0.56767 (16)	0.02352 (15)	0.60617 (15)	0.0213 (4)	
H13A	0.586413	0.007641	0.535122	0.026*	
H13B	0.548205	0.100566	0.597793	0.026*	
C14	0.50120 (16)	−0.14575 (16)	0.67457 (15)	0.0220 (4)	
H14A	0.518813	−0.163034	0.604076	0.026*	
H14B	0.437746	−0.181983	0.712554	0.026*	
C15	0.44349 (16)	−0.00438 (15)	0.76983 (15)	0.0205 (4)	
H15A	0.378951	−0.038674	0.808307	0.025*	
H15B	0.423192	0.072471	0.762594	0.025*	
C16	0.69351 (16)	−0.12818 (15)	0.67461 (15)	0.0208 (4)	
H16A	0.758527	−0.153184	0.712455	0.025*	
H16B	0.713010	−0.144866	0.603934	0.025*	
N21	0.96389 (13)	0.53277 (12)	0.66888 (12)	0.0185 (3)	

N22	1.03238 (14)	0.51130 (13)	0.84249 (13)	0.0209 (3)
N23	0.83260 (14)	0.50888 (13)	0.83676 (13)	0.0211 (3)
N24	0.91408 (14)	0.67678 (13)	0.77182 (13)	0.0207 (3)
C21	0.86158 (16)	0.48569 (15)	0.72915 (15)	0.0206 (4)
H21A	0.798587	0.514069	0.689148	0.025*
H21B	0.874416	0.408596	0.735116	0.025*
C22	0.81436 (16)	0.62564 (15)	0.82683 (16)	0.0221 (4)
H22A	0.794956	0.641618	0.897807	0.027*
H22B	0.751325	0.655797	0.787314	0.027*
C23	1.00907 (16)	0.62886 (15)	0.83182 (16)	0.0226 (4)
H23A	0.992555	0.645241	0.902716	0.027*
H23B	1.075775	0.660737	0.795445	0.027*
C24	1.05778 (16)	0.48863 (15)	0.73384 (15)	0.0201 (4)
H24A	1.073004	0.411640	0.739378	0.024*
H24B	1.125119	0.519334	0.697337	0.024*
C25	0.94127 (16)	0.65112 (14)	0.66518 (15)	0.0205 (4)
H25A	1.007066	0.683951	0.627731	0.025*
H25B	0.879088	0.681840	0.624686	0.025*
C26	0.92924 (16)	0.46570 (15)	0.89559 (15)	0.0217 (4)
H26A	0.942690	0.388452	0.902783	0.026*
H26B	0.911220	0.480513	0.967089	0.026*
N31	0.41819 (13)	0.34324 (13)	0.86223 (13)	0.0213 (3)
N32	0.34067 (15)	0.51211 (14)	0.75097 (14)	0.0266 (4)
N33	0.47210 (17)	0.51353 (15)	0.87450 (15)	0.0325 (4)
N34	0.53923 (15)	0.44041 (15)	0.71314 (14)	0.0289 (4)
C31	0.31950 (17)	0.40495 (16)	0.81169 (17)	0.0266 (4)
H31A	0.299473	0.365307	0.763932	0.032*
H31B	0.255972	0.411911	0.867126	0.032*
C32	0.3720 (2)	0.56912 (17)	0.82560 (18)	0.0329 (5)
H32A	0.386349	0.640567	0.787339	0.040*
H32B	0.309371	0.576543	0.881808	0.040*
C33	0.56536 (19)	0.50044 (19)	0.78861 (19)	0.0349 (5)
H33A	0.631573	0.462773	0.820177	0.042*
H33B	0.582728	0.570673	0.749263	0.042*
C34	0.51269 (18)	0.33500 (16)	0.77563 (16)	0.0272 (4)
H34A	0.578777	0.295933	0.806522	0.033*
H34B	0.494052	0.294447	0.727982	0.033*
C35	0.43694 (18)	0.49921 (17)	0.66807 (17)	0.0291 (4)
H35A	0.452907	0.569471	0.627554	0.035*
H35B	0.417450	0.460785	0.618972	0.035*
C36	0.44831 (19)	0.40664 (17)	0.93320 (16)	0.0275 (4)
H36A	0.386711	0.413627	0.990439	0.033*
H36B	0.514013	0.368715	0.965490	0.033*
N41	0.98222 (14)	0.16814 (13)	0.66156 (13)	0.0236 (3)
N42	1.07891 (16)	−0.00576 (15)	0.62924 (17)	0.0350 (4)
N43	1.09861 (17)	0.05352 (15)	0.79123 (17)	0.0379 (5)
N44	0.92004 (15)	0.00149 (14)	0.77178 (14)	0.0276 (4)
C41	1.04120 (19)	0.10589 (18)	0.58097 (18)	0.0316 (5)

H41A	0.990963	0.107214	0.529629	0.038*
H41B	1.105888	0.139850	0.542356	0.038*
C42	1.15409 (19)	−0.00508 (19)	0.7069 (2)	0.0420 (6)
H42A	1.219661	0.028026	0.669308	0.050*
H42B	1.179667	−0.078443	0.740249	0.050*
C43	0.9988 (2)	0.00220 (19)	0.84575 (19)	0.0358 (5)
H43A	1.022883	−0.071033	0.880625	0.043*
H43B	0.960481	0.040129	0.900804	0.043*
C44	0.88530 (17)	0.11291 (16)	0.71995 (17)	0.0260 (4)
H44A	0.845718	0.151596	0.773986	0.031*
H44B	0.833555	0.113901	0.670081	0.031*
C45	1.0595 (2)	0.16406 (17)	0.7394 (2)	0.0348 (5)
H45A	1.124033	0.199417	0.702869	0.042*
H45B	1.021402	0.202857	0.793862	0.042*
C46	0.98007 (19)	−0.05437 (17)	0.68850 (19)	0.0326 (5)
H46A	0.928905	−0.054578	0.638482	0.039*
H46B	1.003704	−0.128358	0.721415	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0194 (2)	0.0162 (2)	0.0148 (2)	−0.00317 (15)	−0.00286 (15)	−0.00303 (15)
Co2	0.0223 (2)	0.0144 (2)	0.0185 (2)	0.00176 (16)	−0.00397 (16)	−0.00022 (16)
N1	0.0246 (8)	0.0200 (7)	0.0189 (7)	−0.0060 (6)	−0.0018 (6)	−0.0045 (6)
C1	0.0258 (9)	0.0193 (9)	0.0184 (9)	−0.0004 (7)	−0.0006 (7)	−0.0029 (7)
S1	0.0345 (3)	0.0400 (3)	0.0532 (4)	−0.0172 (2)	0.0012 (3)	−0.0224 (3)
N2	0.0247 (8)	0.0206 (8)	0.0232 (8)	0.0042 (6)	−0.0050 (6)	−0.0025 (6)
C2	0.0267 (10)	0.0226 (9)	0.0199 (9)	−0.0029 (8)	−0.0031 (7)	−0.0075 (7)
S2	0.0283 (3)	0.0407 (3)	0.0403 (3)	0.0136 (2)	−0.0156 (2)	−0.0217 (2)
O1	0.0244 (7)	0.0192 (6)	0.0222 (6)	−0.0027 (5)	−0.0082 (5)	−0.0030 (5)
C3	0.0272 (10)	0.0309 (11)	0.0322 (11)	−0.0013 (8)	−0.0083 (8)	−0.0091 (9)
C4	0.0190 (11)	0.0222 (12)	0.0184 (11)	−0.0034 (10)	−0.0006 (8)	−0.0044 (10)
C4′	0.042 (7)	0.059 (10)	0.040 (7)	−0.022 (7)	−0.012 (6)	0.006 (7)
O2	0.0187 (17)	0.0192 (8)	0.0251 (10)	0.0002 (16)	−0.0061 (15)	−0.0012 (7)
O3	0.0245 (10)	0.0260 (9)	0.0324 (10)	−0.0041 (7)	−0.0003 (7)	−0.0087 (7)
C5	0.0244 (13)	0.0246 (12)	0.0298 (13)	−0.0041 (10)	−0.0060 (10)	−0.0004 (10)
C6	0.0291 (13)	0.0293 (13)	0.0308 (14)	−0.0040 (11)	−0.0050 (11)	−0.0052 (11)
O4	0.0187 (17)	0.0192 (8)	0.0251 (10)	0.0002 (16)	−0.0061 (15)	−0.0012 (7)
C7	0.013 (5)	0.028 (5)	0.035 (5)	0.003 (4)	0.002 (4)	−0.008 (4)
C8	0.032 (6)	0.024 (5)	0.028 (5)	−0.001 (4)	−0.006 (4)	0.007 (4)
N11	0.0173 (7)	0.0173 (7)	0.0149 (7)	−0.0003 (6)	−0.0035 (5)	−0.0016 (6)
N12	0.0233 (8)	0.0198 (7)	0.0168 (7)	0.0004 (6)	−0.0046 (6)	−0.0051 (6)
N13	0.0207 (8)	0.0226 (8)	0.0175 (7)	0.0011 (6)	−0.0057 (6)	−0.0060 (6)
N14	0.0203 (7)	0.0204 (8)	0.0154 (7)	−0.0004 (6)	−0.0030 (6)	−0.0041 (6)
C11	0.0247 (9)	0.0165 (8)	0.0163 (8)	−0.0009 (7)	−0.0039 (7)	−0.0033 (7)
C12	0.0204 (9)	0.0208 (9)	0.0152 (8)	−0.0024 (7)	−0.0023 (7)	−0.0033 (7)
C13	0.0233 (9)	0.0225 (9)	0.0165 (8)	0.0017 (7)	−0.0057 (7)	−0.0022 (7)
C14	0.0227 (9)	0.0242 (9)	0.0214 (9)	−0.0016 (7)	−0.0064 (7)	−0.0076 (7)

C15	0.0193 (9)	0.0237 (9)	0.0188 (9)	0.0012 (7)	−0.0044 (7)	−0.0067 (7)
C16	0.0194 (9)	0.0222 (9)	0.0199 (9)	0.0026 (7)	−0.0042 (7)	−0.0053 (7)
N21	0.0185 (7)	0.0153 (7)	0.0200 (7)	−0.0003 (6)	−0.0041 (6)	−0.0004 (6)
N22	0.0226 (8)	0.0189 (7)	0.0209 (8)	0.0001 (6)	−0.0060 (6)	−0.0031 (6)
N23	0.0215 (8)	0.0212 (8)	0.0197 (8)	−0.0026 (6)	−0.0032 (6)	−0.0024 (6)
N24	0.0226 (8)	0.0186 (7)	0.0198 (8)	−0.0002 (6)	−0.0033 (6)	−0.0032 (6)
C21	0.0208 (9)	0.0192 (9)	0.0210 (9)	−0.0024 (7)	−0.0036 (7)	−0.0023 (7)
C22	0.0197 (9)	0.0217 (9)	0.0232 (9)	0.0012 (7)	−0.0032 (7)	−0.0041 (7)
C23	0.0232 (9)	0.0202 (9)	0.0251 (9)	−0.0020 (7)	−0.0073 (7)	−0.0041 (7)
C24	0.0192 (8)	0.0188 (8)	0.0210 (9)	0.0008 (7)	−0.0044 (7)	−0.0028 (7)
C25	0.0246 (9)	0.0154 (8)	0.0197 (9)	−0.0004 (7)	−0.0031 (7)	−0.0014 (7)
C26	0.0239 (9)	0.0197 (9)	0.0196 (9)	−0.0017 (7)	−0.0049 (7)	0.0003 (7)
N31	0.0206 (8)	0.0206 (8)	0.0227 (8)	−0.0029 (6)	−0.0045 (6)	−0.0032 (6)
N32	0.0251 (8)	0.0217 (8)	0.0312 (9)	−0.0001 (7)	−0.0056 (7)	−0.0025 (7)
N33	0.0441 (11)	0.0273 (9)	0.0303 (9)	−0.0127 (8)	−0.0096 (8)	−0.0056 (7)
N34	0.0246 (8)	0.0307 (9)	0.0258 (9)	−0.0009 (7)	−0.0019 (7)	0.0022 (7)
C31	0.0219 (9)	0.0241 (10)	0.0332 (11)	−0.0022 (8)	−0.0071 (8)	−0.0027 (8)
C32	0.0431 (13)	0.0203 (10)	0.0345 (11)	−0.0020 (9)	−0.0035 (9)	−0.0068 (8)
C33	0.0317 (11)	0.0337 (11)	0.0385 (12)	−0.0148 (9)	−0.0111 (9)	0.0056 (9)
C34	0.0277 (10)	0.0249 (10)	0.0251 (10)	0.0040 (8)	−0.0026 (8)	−0.0031 (8)
C35	0.0299 (11)	0.0288 (10)	0.0247 (10)	0.0005 (8)	−0.0057 (8)	0.0007 (8)
C36	0.0343 (11)	0.0281 (10)	0.0221 (9)	−0.0087 (8)	−0.0045 (8)	−0.0054 (8)
N41	0.0239 (8)	0.0223 (8)	0.0236 (8)	−0.0054 (6)	−0.0049 (6)	0.0000 (6)
N42	0.0301 (10)	0.0273 (9)	0.0417 (11)	0.0018 (7)	0.0013 (8)	−0.0037 (8)
N43	0.0397 (11)	0.0287 (10)	0.0452 (11)	−0.0112 (8)	−0.0241 (9)	0.0100 (8)
N44	0.0273 (9)	0.0219 (8)	0.0310 (9)	−0.0063 (7)	−0.0025 (7)	0.0009 (7)
C41	0.0304 (11)	0.0307 (11)	0.0281 (10)	−0.0011 (9)	0.0019 (8)	−0.0010 (9)
C42	0.0240 (11)	0.0309 (12)	0.0623 (17)	−0.0016 (9)	−0.0088 (10)	0.0084 (11)
C43	0.0447 (13)	0.0295 (11)	0.0302 (11)	−0.0087 (10)	−0.0126 (10)	0.0075 (9)
C44	0.0246 (10)	0.0231 (9)	0.0276 (10)	−0.0028 (8)	−0.0034 (8)	−0.0004 (8)
C45	0.0420 (13)	0.0243 (10)	0.0404 (12)	−0.0122 (9)	−0.0219 (10)	0.0056 (9)
C46	0.0343 (11)	0.0199 (10)	0.0434 (13)	−0.0050 (8)	−0.0042 (10)	−0.0059 (9)

Geometric parameters (Å, º)

Co1—N1^{i}	2.0590 (16)	C16—H16B	0.9700
Co1—N1	2.0590 (16)	N21—C21	1.493 (2)
Co1—O1^{i}	2.1388 (13)	N21—C24	1.490 (2)
Co1—O1	2.1388 (13)	N21—C25	1.500 (2)
Co1—N11^{i}	2.2834 (15)	N22—C23	1.478 (2)
Co1—N11	2.2834 (15)	N22—C24	1.474 (2)
Co2—N2^{ii}	2.0812 (16)	N22—C26	1.469 (2)
Co2—N2	2.0812 (16)	N23—C21	1.465 (2)
Co2—O2	2.029 (6)	N23—C22	1.468 (2)
Co2—O2^{ii}	2.029 (6)	N23—C26	1.469 (2)
Co2—O4^{ii}	2.21 (3)	N24—C22	1.473 (2)
Co2—O4	2.21 (3)	N24—C23	1.470 (2)
Co2—N21	2.2788 (16)	N24—C25	1.465 (2)

Co2—N21^{ii}	2.2788 (16)	C21—H21A	0.9700
N1—C1	1.169 (3)	C21—H21B	0.9700
C1—S1	1.629 (2)	C22—H22A	0.9700
N2—C2	1.154 (3)	C22—H22B	0.9700
C2—S2	1.643 (2)	C23—H23A	0.9700
O1—H1	0.880 (18)	C23—H23B	0.9700
O1—C3	1.464 (2)	C24—H24A	0.9700
C3—H3AA	0.9700	C24—H24B	0.9700
C3—H3AB	0.9700	C25—H25A	0.9700
C3—H3BC	0.9700	C25—H25B	0.9700
C3—H3BD	0.9700	C26—H26A	0.9700
C3—C4	1.515 (3)	C26—H26B	0.9700
C3—C4′	1.4495 (10)	N31—C31	1.486 (2)
C4—H4A	0.9600	N31—C34	1.474 (3)
C4—H4B	0.9600	N31—C36	1.486 (2)
C4—H4C	0.9600	N32—C31	1.466 (3)
C4′—H4′A	0.9600	N32—C32	1.471 (3)
C4′—H4′B	0.9600	N32—C35	1.465 (3)
C4′—H4′C	0.9600	N33—C32	1.469 (3)
O2—H2A	0.872 (19)	N33—C33	1.467 (3)
O2—H2B	0.871 (19)	N33—C36	1.463 (3)
O3—C5	1.433 (3)	N34—C33	1.480 (3)
O3—H3	0.871 (19)	N34—C34	1.470 (3)
C5—H5A	0.9700	N34—C35	1.480 (3)
C5—H5B	0.9700	C31—H31A	0.9700
C5—C6	1.505 (4)	C31—H31B	0.9700
C6—H6A	0.9600	C32—H32A	0.9700
C6—H6B	0.9600	C32—H32B	0.9700
C6—H6C	0.9600	C33—H33A	0.9700
O4—C7	1.427 (17)	C33—H33B	0.9700
O4—H4	0.87 (2)	C34—H34A	0.9700
C7—H7A	0.9700	C34—H34B	0.9700
C7—H7B	0.9700	C35—H35A	0.9700
C7—C8	1.507 (13)	C35—H35B	0.9700
C8—H8A	0.9600	C36—H36A	0.9700
C8—H8B	0.9600	C36—H36B	0.9700
C8—H8C	0.9600	N41—C41	1.483 (3)
N11—C11	1.499 (2)	N41—C44	1.482 (2)
N11—C12	1.488 (2)	N41—C45	1.475 (3)
N11—C15	1.496 (2)	N42—C41	1.465 (3)
N12—C11	1.465 (2)	N42—C42	1.469 (3)
N12—C14	1.472 (2)	N42—C46	1.464 (3)
N12—C16	1.476 (2)	N43—C42	1.479 (4)
N13—C13	1.474 (2)	N43—C43	1.473 (3)
N13—C14	1.470 (2)	N43—C45	1.469 (3)
N13—C15	1.468 (2)	N44—C43	1.465 (3)
N14—C12	1.467 (2)	N44—C44	1.467 (3)
N14—C13	1.472 (2)	N44—C46	1.463 (3)

N14—C16	1.473 (2)	C41—H41A	0.9700
C11—H11A	0.9700	C41—H41B	0.9700
C11—H11B	0.9700	C42—H42A	0.9700
C12—H12A	0.9700	C42—H42B	0.9700
C12—H12B	0.9700	C43—H43A	0.9700
C13—H13A	0.9700	C43—H43B	0.9700
C13—H13B	0.9700	C44—H44A	0.9700
C14—H14A	0.9700	C44—H44B	0.9700
C14—H14B	0.9700	C45—H45A	0.9700
C15—H15A	0.9700	C45—H45B	0.9700
C15—H15B	0.9700	C46—H46A	0.9700
C16—H16A	0.9700	C46—H46B	0.9700

N1^{i}—Co1—N1	180.0	N14—C16—H16A	109.1
N1—Co1—O1^{i}	89.16 (6)	N14—C16—H16B	109.1
N1^{i}—Co1—O1	89.16 (6)	H16A—C16—H16B	107.9
N1—Co1—O1	90.84 (6)	C21—N21—Co2	110.79 (11)
N1^{i}—Co1—O1^{i}	90.84 (6)	C21—N21—C25	106.97 (14)
N1^{i}—Co1—N11	93.90 (6)	C24—N21—Co2	113.66 (11)
N1—Co1—N11	86.10 (6)	C24—N21—C21	107.30 (14)
N1—Co1—N11^{i}	93.90 (6)	C24—N21—C25	107.16 (14)
N1^{i}—Co1—N11^{i}	86.10 (6)	C25—N21—Co2	110.66 (11)
O1—Co1—O1^{i}	180.00 (7)	C24—N22—C23	108.01 (14)
O1^{i}—Co1—N11^{i}	91.57 (5)	C26—N22—C23	107.79 (15)
O1—Co1—N11	91.57 (5)	C26—N22—C24	108.16 (15)
O1—Co1—N11^{i}	88.43 (5)	C21—N23—C22	108.62 (14)
O1^{i}—Co1—N11	88.43 (5)	C21—N23—C26	108.13 (15)
N11—Co1—N11^{i}	180.0	C22—N23—C26	107.86 (15)
N2—Co2—N2^{ii}	180.0	C23—N24—C22	108.30 (14)
N2—Co2—O4	85.7 (7)	C25—N24—C22	107.77 (15)
N2^{ii}—Co2—O4^{ii}	85.7 (7)	C25—N24—C23	107.98 (15)
N2—Co2—O4^{ii}	94.3 (7)	N21—C21—H21A	109.1
N2^{ii}—Co2—O4	94.3 (7)	N21—C21—H21B	109.1
N2—Co2—N21^{ii}	91.78 (6)	N23—C21—N21	112.54 (15)
N2^{ii}—Co2—N21^{ii}	88.22 (6)	N23—C21—H21A	109.1
N2^{ii}—Co2—N21	91.78 (6)	N23—C21—H21B	109.1
N2—Co2—N21	88.22 (6)	H21A—C21—H21B	107.8
O2^{ii}—Co2—N2	89.20 (16)	N23—C22—N24	112.53 (15)
O2—Co2—N2^{ii}	89.20 (16)	N23—C22—H22A	109.1
O2^{ii}—Co2—N2^{ii}	90.80 (16)	N23—C22—H22B	109.1
O2—Co2—N2	90.80 (16)	N24—C22—H22A	109.1
O2^{ii}—Co2—O2	180.0	N24—C22—H22B	109.1
O2—Co2—O4^{ii}	174.6 (9)	H22A—C22—H22B	107.8
O2^{ii}—Co2—O4^{ii}	5.4 (9)	N22—C23—H23A	109.1
O2—Co2—N21	91.3 (2)	N22—C23—H23B	109.1
O2—Co2—N21^{ii}	88.7 (2)	N24—C23—N22	112.47 (15)
O2^{ii}—Co2—N21^{ii}	91.3 (2)	N24—C23—H23A	109.1
O2^{ii}—Co2—N21	88.7 (2)	N24—C23—H23B	109.1

O4^{ii}—Co2—O4	180.0	H23A—C23—H23B	107.8
O4^{ii}—Co2—N21^{ii}	92.9 (9)	N21—C24—H24A	109.1
O4—Co2—N21	92.9 (9)	N21—C24—H24B	109.1
O4^{ii}—Co2—N21	87.1 (9)	N22—C24—N21	112.52 (15)
O4—Co2—N21^{ii}	87.1 (9)	N22—C24—H24A	109.1
N21^{ii}—Co2—N21	180.0	N22—C24—H24B	109.1
C1—N1—Co1	164.85 (15)	H24A—C24—H24B	107.8
N1—C1—S1	178.89 (18)	N21—C25—H25A	109.0
C2—N2—Co2	175.29 (16)	N21—C25—H25B	109.0
N2—C2—S2	177.31 (19)	N24—C25—N21	112.98 (14)
Co1—O1—H1	122 (2)	N24—C25—H25A	109.0
C3—O1—Co1	129.84 (12)	N24—C25—H25B	109.0
C3—O1—H1	107 (2)	H25A—C25—H25B	107.8
O1—C3—H3AA	109.0	N22—C26—H26A	109.0
O1—C3—H3AB	109.0	N22—C26—H26B	109.0
O1—C3—H3BC	106.0	N23—C26—N22	112.80 (15)
O1—C3—H3BD	106.0	N23—C26—H26A	109.0
O1—C3—C4	113.01 (18)	N23—C26—H26B	109.0
H3AA—C3—H3AB	107.8	H26A—C26—H26B	107.8
H3BC—C3—H3BD	106.3	C34—N31—C31	107.28 (15)
C4—C3—H3AA	109.0	C34—N31—C36	107.97 (16)
C4—C3—H3AB	109.0	C36—N31—C31	107.86 (16)
C4′—C3—O1	125.1 (6)	C31—N32—C32	107.40 (17)
C4′—C3—H3BC	106.0	C35—N32—C31	107.85 (16)
C4′—C3—H3BD	106.0	C35—N32—C32	108.44 (17)
C3—C4—H4A	109.5	C33—N33—C32	108.52 (17)
C3—C4—H4B	109.5	C36—N33—C32	108.32 (17)
C3—C4—H4C	109.5	C36—N33—C33	108.01 (18)
H4A—C4—H4B	109.5	C34—N34—C33	107.50 (16)
H4A—C4—H4C	109.5	C34—N34—C35	108.18 (16)
H4B—C4—H4C	109.5	C35—N34—C33	107.51 (17)
C3—C4′—H4′A	109.5	N31—C31—H31A	109.0
C3—C4′—H4′B	109.5	N31—C31—H31B	109.0
C3—C4′—H4′C	109.5	N32—C31—N31	112.86 (16)
H4′A—C4′—H4′B	109.5	N32—C31—H31A	109.0
H4′A—C4′—H4′C	109.5	N32—C31—H31B	109.0
H4′B—C4′—H4′C	109.5	H31A—C31—H31B	107.8
Co2—O2—H2A	127 (4)	N32—C32—H32A	109.1
Co2—O2—H2B	123 (3)	N32—C32—H32B	109.1
H2A—O2—H2B	106 (4)	N33—C32—N32	112.59 (17)
C5—O3—H3	112 (3)	N33—C32—H32A	109.1
O3—C5—H5A	109.8	N33—C32—H32B	109.1
O3—C5—H5B	109.8	H32A—C32—H32B	107.8
O3—C5—C6	109.6 (2)	N33—C33—N34	112.55 (17)
H5A—C5—H5B	108.2	N33—C33—H33A	109.1
C6—C5—H5A	109.8	N33—C33—H33B	109.1
C6—C5—H5B	109.8	N34—C33—H33A	109.1
C5—C6—H6A	109.5	N34—C33—H33B	109.1

C5—C6—H6B	109.5	H33A—C33—H33B	107.8
C5—C6—H6C	109.5	N31—C34—H34A	109.1
H6A—C6—H6B	109.5	N31—C34—H34B	109.1
H6A—C6—H6C	109.5	N34—C34—N31	112.62 (16)
H6B—C6—H6C	109.5	N34—C34—H34A	109.1
Co2—O4—H4	115 (10)	N34—C34—H34B	109.1
C7—O4—Co2	137 (2)	H34A—C34—H34B	107.8
C7—O4—H4	106 (10)	N32—C35—N34	112.61 (16)
O4—C7—H7A	109.1	N32—C35—H35A	109.1
O4—C7—H7B	109.1	N32—C35—H35B	109.1
O4—C7—C8	112.4 (15)	N34—C35—H35A	109.1
H7A—C7—H7B	107.9	N34—C35—H35B	109.1
C8—C7—H7A	109.1	H35A—C35—H35B	107.8
C8—C7—H7B	109.1	N31—C36—H36A	109.2
C7—C8—H8A	109.5	N31—C36—H36B	109.2
C7—C8—H8B	109.5	N33—C36—N31	111.87 (16)
C7—C8—H8C	109.5	N33—C36—H36A	109.2
H8A—C8—H8B	109.5	N33—C36—H36B	109.2
H8A—C8—H8C	109.5	H36A—C36—H36B	107.9
H8B—C8—H8C	109.5	C44—N41—C41	107.46 (16)
C11—N11—Co1	112.38 (10)	C45—N41—C41	108.17 (18)
C12—N11—Co1	110.45 (11)	C45—N41—C44	107.65 (16)
C12—N11—C11	106.96 (14)	C41—N42—C42	107.76 (19)
C12—N11—C15	106.95 (13)	C46—N42—C41	107.89 (17)
C15—N11—Co1	112.93 (11)	C46—N42—C42	107.80 (19)
C15—N11—C11	106.83 (14)	C43—N43—C42	107.73 (19)
C11—N12—C14	108.22 (14)	C45—N43—C42	108.42 (19)
C11—N12—C16	108.09 (14)	C45—N43—C43	107.79 (19)
C14—N12—C16	108.03 (14)	C43—N44—C44	108.03 (17)
C14—N13—C13	107.97 (15)	C46—N44—C43	108.19 (18)
C15—N13—C13	107.82 (14)	C46—N44—C44	107.81 (16)
C15—N13—C14	108.50 (14)	N41—C41—H41A	109.1
C12—N14—C13	108.45 (14)	N41—C41—H41B	109.1
C12—N14—C16	108.30 (14)	N42—C41—N41	112.64 (17)
C13—N14—C16	107.44 (14)	N42—C41—H41A	109.1
N11—C11—H11A	109.0	N42—C41—H41B	109.1
N11—C11—H11B	109.0	H41A—C41—H41B	107.8
N12—C11—N11	113.01 (14)	N42—C42—N43	112.48 (18)
N12—C11—H11A	109.0	N42—C42—H42A	109.1
N12—C11—H11B	109.0	N42—C42—H42B	109.1
H11A—C11—H11B	107.8	N43—C42—H42A	109.1
N11—C12—H12A	109.0	N43—C42—H42B	109.1
N11—C12—H12B	109.0	H42A—C42—H42B	107.8
N14—C12—N11	112.97 (15)	N43—C43—H43A	109.1
N14—C12—H12A	109.0	N43—C43—H43B	109.1
N14—C12—H12B	109.0	N44—C43—N43	112.46 (18)
H12A—C12—H12B	107.8	N44—C43—H43A	109.1
N13—C13—H13A	109.1	N44—C43—H43B	109.1

N13—C13—H13B	109.1	H43A—C43—H43B	107.8
N14—C13—N13	112.61 (14)	N41—C44—H44A	109.1
N14—C13—H13A	109.1	N41—C44—H44B	109.1
N14—C13—H13B	109.1	N44—C44—N41	112.30 (16)
H13A—C13—H13B	107.8	N44—C44—H44A	109.1
N12—C14—H14A	109.1	N44—C44—H44B	109.1
N12—C14—H14B	109.1	H44A—C44—H44B	107.9
N13—C14—N12	112.35 (15)	N41—C45—H45A	109.2
N13—C14—H14A	109.1	N41—C45—H45B	109.2
N13—C14—H14B	109.1	N43—C45—N41	112.17 (17)
H14A—C14—H14B	107.9	N43—C45—H45A	109.2
N11—C15—H15A	109.0	N43—C45—H45B	109.2
N11—C15—H15B	109.0	H45A—C45—H45B	107.9
N13—C15—N11	112.95 (14)	N42—C46—H46A	108.9
N13—C15—H15A	109.0	N42—C46—H46B	108.9
N13—C15—H15B	109.0	N44—C46—N42	113.21 (17)
H15A—C15—H15B	107.8	N44—C46—H46A	108.9
N12—C16—H16A	109.1	N44—C46—H46B	108.9
N12—C16—H16B	109.1	H46A—C46—H46B	107.7
N14—C16—N12	112.42 (15)		

Co1—O1—C3—C4	121.56 (18)	C26—N22—C23—N24	−57.6 (2)
Co1—O1—C3—C4′	85.5 (9)	C26—N22—C24—N21	57.87 (19)
Co1—N11—C11—N12	−178.62 (11)	C26—N23—C21—N21	−58.52 (19)
Co1—N11—C12—N14	179.71 (11)	C26—N23—C22—N24	58.1 (2)
Co1—N11—C15—N13	179.36 (12)	C31—N31—C34—N34	57.9 (2)
Co2—O4—C7—C8	125 (2)	C31—N31—C36—N33	−57.3 (2)
Co2—N21—C21—N23	−177.58 (11)	C31—N32—C32—N33	58.9 (2)
Co2—N21—C24—N22	179.79 (11)	C31—N32—C35—N34	−58.0 (2)
Co2—N21—C25—N24	178.24 (12)	C32—N32—C31—N31	−58.1 (2)
C11—N11—C12—N14	57.12 (18)	C32—N32—C35—N34	58.0 (2)
C11—N11—C15—N13	−56.60 (19)	C32—N33—C33—N34	−57.9 (2)
C11—N12—C14—N13	58.77 (19)	C32—N33—C36—N31	58.5 (2)
C11—N12—C16—N14	−58.43 (18)	C33—N33—C32—N32	57.4 (2)
C12—N11—C11—N12	−57.24 (19)	C33—N33—C36—N31	−58.9 (2)
C12—N11—C15—N13	57.65 (19)	C33—N34—C34—N31	57.9 (2)
C12—N14—C13—N13	−58.23 (19)	C33—N34—C35—N32	−58.0 (2)
C12—N14—C16—N12	58.46 (19)	C34—N31—C31—N32	−58.4 (2)
C13—N13—C14—N12	58.01 (19)	C34—N31—C36—N33	58.3 (2)
C13—N13—C15—N11	−58.61 (19)	C34—N34—C33—N33	−58.4 (2)
C13—N14—C12—N11	57.91 (19)	C34—N34—C35—N32	57.8 (2)
C13—N14—C16—N12	−58.50 (19)	C35—N32—C31—N31	58.6 (2)
C14—N12—C11—N11	−58.54 (19)	C35—N32—C32—N33	−57.4 (2)
C14—N12—C16—N14	58.45 (19)	C35—N34—C33—N33	57.9 (2)
C14—N13—C13—N14	−58.58 (19)	C35—N34—C34—N31	−58.0 (2)
C14—N13—C15—N11	58.09 (19)	C36—N31—C31—N32	57.7 (2)
C15—N11—C11—N12	57.00 (19)	C36—N31—C34—N34	−58.1 (2)
C15—N11—C12—N14	−57.03 (18)	C36—N33—C32—N32	−59.6 (2)

C15—N13—C13—N14	58.46 (19)	C36—N33—C33—N34	59.3 (2)
C15—N13—C14—N12	−58.6 (2)	C41—N41—C44—N44	58.1 (2)
C16—N12—C11—N11	58.22 (19)	C41—N41—C45—N43	−57.3 (2)
C16—N12—C14—N13	−58.04 (19)	C41—N42—C42—N43	58.4 (2)
C16—N14—C12—N11	−58.39 (19)	C41—N42—C46—N44	−58.3 (2)
C16—N14—C13—N13	58.63 (19)	C42—N42—C41—N41	−58.4 (2)
C21—N21—C24—N22	−57.37 (19)	C42—N42—C46—N44	57.9 (2)
C21—N21—C25—N24	57.47 (19)	C42—N43—C43—N44	−58.0 (2)
C21—N23—C22—N24	−58.9 (2)	C42—N43—C45—N41	57.5 (2)
C21—N23—C26—N22	58.7 (2)	C43—N43—C42—N42	58.1 (2)
C22—N23—C21—N21	58.28 (19)	C43—N43—C45—N41	−58.8 (3)
C22—N23—C26—N22	−58.6 (2)	C43—N44—C44—N41	58.3 (2)
C22—N24—C23—N22	57.5 (2)	C43—N44—C46—N42	−57.9 (2)
C22—N24—C25—N21	−58.47 (19)	C44—N41—C41—N42	−57.8 (2)
C23—N22—C24—N21	−58.54 (19)	C44—N41—C45—N43	58.5 (2)
C23—N22—C26—N23	58.2 (2)	C44—N44—C43—N43	−58.6 (2)
C23—N24—C22—N23	−57.9 (2)	C44—N44—C46—N42	58.7 (2)
C23—N24—C25—N21	58.31 (19)	C45—N41—C41—N42	58.1 (2)
C24—N21—C21—N23	57.83 (19)	C45—N41—C44—N44	−58.2 (2)
C24—N21—C25—N24	−57.34 (19)	C45—N43—C42—N42	−58.3 (2)
C24—N22—C23—N24	59.1 (2)	C45—N43—C43—N44	58.8 (3)
C24—N22—C26—N23	−58.31 (19)	C46—N42—C41—N41	57.7 (2)
C25—N21—C21—N23	−56.89 (18)	C46—N42—C42—N43	−57.8 (2)
C25—N21—C24—N22	57.21 (19)	C46—N44—C43—N43	57.8 (2)
C25—N24—C22—N23	58.72 (19)	C46—N44—C44—N41	−58.4 (2)
C25—N24—C23—N22	−58.9 (2)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N31	0.88 (2)	1.92 (2)	2.793 (2)	170 (3)
C4′—H4′*A*···N43^{iii}	0.96	2.50	3.243 (14)	134
C4′—H4′*C*···N44^{i}	0.96	2.38	3.161 (10)	138
O2—H2*A*···N41	0.87 (2)	1.88 (2)	2.743 (7)	173 (7)
O2—H2*B*···O3	0.87 (2)	1.80 (2)	2.665 (4)	177 (5)
C5—H5*A*···S2^{iv}	0.97	3.02	3.925 (3)	156
O3—H3···N34	0.87 (2)	1.97 (2)	2.821 (3)	167 (4)
O4—H4···N41	0.87 (2)	1.94 (5)	2.81 (3)	170 (19)
C11—H11*A*···O1^{i}	0.97	2.49	3.058 (2)	117
C11—H11*B*···N1	0.97	2.67	3.213 (2)	116
C12—H12*B*···N44	0.97	2.64	3.423 (3)	138
C13—H13*A*···N13^{v}	0.97	2.70	3.563 (2)	149
C13—H13*B*···S2^{iv}	0.97	2.95	3.7150 (19)	136
C14—H14*A*···S2^{vi}	0.97	2.93	3.840 (2)	156
C15—H15*B*···O1	0.97	2.61	3.118 (2)	113
C22—H22*B*···N12^{vii}	0.97	2.58	3.448 (2)	149

C25—H25*A*···O2^{ii}	0.97	2.50	3.026 (7)	114
C25—H25*A*···O4^{ii}	0.97	2.49	3.08 (3)	119
C25—H25*B*···N2	0.97	2.61	3.202 (3)	119
C26—H26*A*···S1^{i}	0.97	2.98	3.655 (2)	128
C26—H26*B*···N22^{viii}	0.97	2.69	3.581 (3)	152
C33—H33*A*···N23	0.97	2.66	3.431 (3)	137
C45—H45*A*···S2^{ii}	0.97	3.01	3.959 (3)	165

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*, *y*−1, *z*; (vii) *x*, *y*+1, *z*; (viii) −*x*+2, −*y*+1, −*z*+2.

\ Tris(ethanol-*κO*)(hexamethylenetetramine-*κN*)bis(thiocyanato-\ *κN*)cobalt(II) (2)

Crystal data

$[Co(NCS)_2(C_6H_{12}N_4)(C_2H_6O)_3]$
M_r = 453.49
Monoclinic, $P2_1/n$
a = 11.1463 (1) Å
b = 15.7705 (1) Å
c = 12.1824 (1) Å
β = 103.886 (1)°
V = 2078.87 (3) Å^3
Z = 4
$F(000)$ = 956
D_x = 1.449 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 23697 reflections
θ = 4.7–78.0°
μ = 8.57 mm^{-1}
T = 100 K
Block, intense orange
0.2 × 0.18 × 0.03 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.427, T_{max} = 1.000
29441 measured reflections
4431 independent reflections
4373 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 78.2°, θ_{min} = 4.7°
h = −14→13
k = −20→18
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.068
S = 1.08
4431 reflections
242 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.8765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: SHELXL2016/6 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00065 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.51335 (2)	0.27266 (2)	0.57458 (2)	0.01059 (7)
N1	0.67247 (10)	0.34371 (7)	0.62465 (9)	0.0153 (2)
C1	0.76466 (12)	0.38035 (8)	0.65618 (11)	0.0141 (2)
S1	0.89474 (3)	0.43141 (2)	0.70092 (3)	0.02407 (10)
N2	0.35462 (10)	0.20093 (7)	0.52823 (9)	0.0153 (2)
C2	0.25674 (12)	0.17255 (8)	0.49267 (11)	0.0134 (2)
S2	0.11817 (3)	0.13335 (2)	0.44031 (3)	0.01552 (8)
N11	0.48544 (9)	0.32562 (7)	0.39886 (9)	0.0110 (2)
N12	0.35142 (10)	0.34740 (7)	0.20867 (9)	0.0131 (2)
N13	0.49385 (10)	0.45980 (7)	0.29661 (9)	0.0127 (2)
N14	0.57416 (10)	0.32908 (7)	0.23263 (9)	0.0137 (2)
C11	0.36212 (11)	0.30856 (8)	0.32095 (10)	0.0123 (2)
H11A	0.349734	0.246546	0.312045	0.015*
H11B	0.296401	0.331440	0.354686	0.015*
C12	0.37105 (12)	0.44001 (8)	0.22303 (11)	0.0140 (2)
H12A	0.363639	0.466531	0.148044	0.017*
H12B	0.306101	0.464431	0.256487	0.017*
C13	0.58915 (12)	0.42110 (8)	0.24547 (11)	0.0147 (2)
H13A	0.583835	0.446900	0.170375	0.018*
H13B	0.672136	0.433681	0.293783	0.018*
C14	0.58124 (11)	0.29098 (8)	0.34359 (11)	0.0130 (2)
H14A	0.664260	0.301634	0.393063	0.016*
H14B	0.570316	0.228850	0.334757	0.016*
C15	0.45097 (12)	0.31188 (8)	0.15994 (11)	0.0147 (2)
H15A	0.439358	0.249853	0.150305	0.018*
H15B	0.445047	0.337046	0.084374	0.018*
C16	0.50169 (12)	0.41931 (8)	0.40684 (11)	0.0126 (2)
H16A	0.437357	0.443759	0.441062	0.015*
H16B	0.583193	0.432292	0.457605	0.015*
O21	0.41718 (8)	0.37678 (6)	0.62519 (8)	0.01481 (19)
H21	0.458750	0.419051	0.654234	0.022*
C21	0.31119 (12)	0.36740 (9)	0.67299 (12)	0.0174 (3)
H21A	0.320943	0.404600	0.740012	0.021*
H21B	0.306126	0.308048	0.697966	0.021*
C22	0.19389 (14)	0.39014 (12)	0.58774 (14)	0.0295 (3)
H22A	0.181805	0.351233	0.523285	0.044*
H22B	0.199742	0.448405	0.561561	0.044*
H22C	0.123733	0.385578	0.622869	0.044*
O31	0.62924 (8)	0.17312 (6)	0.54561 (8)	0.01390 (18)
H31	0.695985	0.172350	0.595461	0.021*
C31	0.59743 (13)	0.08809 (8)	0.50586 (12)	0.0172 (3)
H31A	0.508810	0.085995	0.466374	0.021*
H31B	0.610588	0.049076	0.571334	0.021*
C32	0.67444 (14)	0.05882 (9)	0.42600 (12)	0.0210 (3)
H32A	0.658634	0.095774	0.359399	0.032*

H32B	0.652206	0.000353	0.402320	0.032*
H32C	0.762264	0.061398	0.464640	0.032*
O41	0.54084 (10)	0.22913 (6)	0.74187 (8)	0.0173 (2)
H41	0.564436	0.261997	0.797094	0.026*
C41	0.51429 (13)	0.14737 (9)	0.78184 (12)	0.0197 (3)
H41A	0.591114	0.123102	0.829704	0.024*
H41B	0.485447	0.109128	0.716372	0.024*
C42	0.41750 (15)	0.15144 (12)	0.84905 (16)	0.0344 (4)
H42A	0.339647	0.171959	0.800591	0.052*
H42B	0.444763	0.190262	0.912993	0.052*
H42C	0.405042	0.094752	0.877347	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00865 (11)	0.01120 (12)	0.01104 (12)	−0.00058 (7)	0.00060 (8)	−0.00032 (7)
N1	0.0121 (5)	0.0164 (5)	0.0155 (5)	−0.0011 (4)	−0.0003 (4)	−0.0007 (4)
C1	0.0149 (6)	0.0116 (6)	0.0154 (6)	0.0034 (5)	0.0029 (5)	0.0009 (5)
S1	0.01192 (16)	0.01850 (17)	0.0400 (2)	−0.00438 (12)	0.00274 (14)	−0.00662 (14)
N2	0.0143 (5)	0.0149 (5)	0.0157 (5)	−0.0015 (4)	0.0016 (4)	0.0008 (4)
C2	0.0157 (6)	0.0123 (6)	0.0122 (5)	0.0019 (5)	0.0035 (5)	0.0015 (4)
S2	0.01174 (15)	0.01751 (16)	0.01595 (15)	−0.00302 (11)	0.00064 (11)	−0.00024 (11)
N11	0.0099 (5)	0.0110 (5)	0.0114 (5)	−0.0007 (4)	0.0014 (4)	−0.0008 (4)
N12	0.0133 (5)	0.0133 (5)	0.0117 (5)	−0.0004 (4)	0.0015 (4)	0.0004 (4)
N13	0.0117 (5)	0.0125 (5)	0.0132 (5)	−0.0006 (4)	0.0018 (4)	0.0005 (4)
N14	0.0135 (5)	0.0143 (5)	0.0137 (5)	−0.0003 (4)	0.0038 (4)	0.0003 (4)
C11	0.0101 (5)	0.0146 (6)	0.0111 (6)	−0.0015 (4)	0.0006 (4)	0.0010 (4)
C12	0.0117 (6)	0.0128 (6)	0.0156 (6)	0.0005 (4)	−0.0003 (5)	0.0017 (5)
C13	0.0126 (6)	0.0150 (6)	0.0169 (6)	−0.0014 (5)	0.0044 (5)	0.0002 (5)
C14	0.0116 (6)	0.0145 (6)	0.0134 (6)	0.0029 (5)	0.0037 (5)	0.0006 (5)
C15	0.0157 (6)	0.0157 (6)	0.0127 (6)	−0.0009 (5)	0.0037 (5)	−0.0018 (5)
C16	0.0131 (6)	0.0115 (6)	0.0124 (5)	−0.0006 (4)	0.0017 (5)	−0.0010 (4)
O21	0.0123 (4)	0.0142 (4)	0.0191 (5)	−0.0019 (3)	0.0062 (4)	−0.0027 (3)
C21	0.0156 (6)	0.0202 (7)	0.0183 (6)	−0.0013 (5)	0.0078 (5)	−0.0025 (5)
C22	0.0155 (7)	0.0410 (9)	0.0313 (8)	0.0045 (6)	0.0044 (6)	−0.0042 (7)
O31	0.0114 (4)	0.0129 (4)	0.0148 (4)	0.0013 (3)	−0.0020 (3)	−0.0017 (3)
C31	0.0169 (6)	0.0139 (6)	0.0190 (6)	−0.0001 (5)	0.0007 (5)	−0.0031 (5)
C32	0.0215 (7)	0.0214 (7)	0.0175 (6)	0.0063 (5)	−0.0008 (5)	−0.0041 (5)
O41	0.0230 (5)	0.0156 (5)	0.0122 (4)	−0.0048 (3)	0.0022 (4)	−0.0001 (3)
C41	0.0209 (7)	0.0159 (6)	0.0192 (6)	−0.0026 (5)	−0.0011 (5)	0.0040 (5)
C42	0.0219 (8)	0.0392 (9)	0.0434 (10)	−0.0028 (7)	0.0103 (7)	0.0176 (8)

Geometric parameters (Å, º)

Co1—N2	2.0615 (11)	C14—H14B	0.9900
Co1—N1	2.0624 (11)	C15—H15A	0.9900
Co1—O41	2.1021 (10)	C15—H15B	0.9900
Co1—O31	2.1157 (9)	C16—H16A	0.9900

Co1—O21	2.1314 (9)	C16—H16B	0.9900
Co1—N11	2.2489 (11)	O21—C21	1.4446 (15)
N1—C1	1.1610 (18)	O21—H21	0.8400
C1—S1	1.6335 (13)	C21—C22	1.505 (2)
N2—C2	1.1625 (18)	C21—H21A	0.9900
C2—S2	1.6437 (13)	C21—H21B	0.9900
N11—C16	1.4889 (16)	C22—H22A	0.9800
N11—C11	1.4955 (15)	C22—H22B	0.9800
N11—C14	1.4957 (15)	C22—H22C	0.9800
N12—C11	1.4771 (15)	O31—C31	1.4409 (16)
N12—C12	1.4810 (16)	O31—H31	0.8400
N12—C15	1.4878 (16)	C31—C32	1.5157 (19)
N13—C16	1.4705 (16)	C31—H31A	0.9900
N13—C12	1.4783 (16)	C31—H31B	0.9900
N13—C13	1.4855 (16)	C32—H32A	0.9800
N14—C14	1.4640 (16)	C32—H32B	0.9800
N14—C13	1.4648 (17)	C32—H32C	0.9800
N14—C15	1.4695 (16)	O41—C41	1.4339 (16)
C11—H11A	0.9900	O41—H41	0.8400
C11—H11B	0.9900	C41—C42	1.504 (2)
C12—H12A	0.9900	C41—H41A	0.9900
C12—H12B	0.9900	C41—H41B	0.9900
C13—H13A	0.9900	C42—H42A	0.9800
C13—H13B	0.9900	C42—H42B	0.9800
C14—H14A	0.9900	C42—H42C	0.9800

N2—Co1—N1	178.73 (4)	N14—C15—N12	111.62 (10)
N2—Co1—O41	90.12 (4)	N14—C15—H15A	109.3
N1—Co1—O41	88.61 (4)	N12—C15—H15A	109.3
N2—Co1—O31	93.75 (4)	N14—C15—H15B	109.3
N1—Co1—O31	86.35 (4)	N12—C15—H15B	109.3
O41—Co1—O31	88.09 (4)	H15A—C15—H15B	108.0
N2—Co1—O21	92.51 (4)	N13—C16—N11	113.06 (10)
N1—Co1—O21	87.27 (4)	N13—C16—H16A	109.0
O41—Co1—O21	86.42 (4)	N11—C16—H16A	109.0
O31—Co1—O21	171.68 (4)	N13—C16—H16B	109.0
N2—Co1—N11	91.69 (4)	N11—C16—H16B	109.0
N1—Co1—N11	89.57 (4)	H16A—C16—H16B	107.8
O41—Co1—N11	177.25 (4)	C21—O21—Co1	123.67 (8)
O31—Co1—N11	93.85 (4)	C21—O21—H21	109.5
O21—Co1—N11	91.43 (4)	Co1—O21—H21	117.9
C1—N1—Co1	176.60 (11)	O21—C21—C22	110.89 (12)
N1—C1—S1	179.67 (14)	O21—C21—H21A	109.5
C2—N2—Co1	168.63 (11)	C22—C21—H21A	109.5
N2—C2—S2	179.00 (12)	O21—C21—H21B	109.5
C16—N11—C11	107.39 (9)	C22—C21—H21B	109.5
C16—N11—C14	107.64 (10)	H21A—C21—H21B	108.0
C11—N11—C14	107.18 (10)	C21—C22—H22A	109.5

C16—N11—Co1	108.63 (7)	C21—C22—H22B	109.5
C11—N11—Co1	115.68 (7)	H22A—C22—H22B	109.5
C14—N11—Co1	110.02 (7)	C21—C22—H22C	109.5
C11—N12—C12	108.83 (10)	H22A—C22—H22C	109.5
C11—N12—C15	108.14 (10)	H22B—C22—H22C	109.5
C12—N12—C15	108.38 (10)	C31—O31—Co1	129.48 (8)
C16—N13—C12	107.78 (10)	C31—O31—H31	109.5
C16—N13—C13	108.23 (10)	Co1—O31—H31	111.1
C12—N13—C13	108.07 (10)	O31—C31—C32	111.56 (11)
C14—N14—C13	109.17 (10)	O31—C31—H31A	109.3
C14—N14—C15	108.43 (10)	C32—C31—H31A	109.3
C13—N14—C15	108.26 (10)	O31—C31—H31B	109.3
N12—C11—N11	111.76 (10)	C32—C31—H31B	109.3
N12—C11—H11A	109.3	H31A—C31—H31B	108.0
N11—C11—H11A	109.3	C31—C32—H32A	109.5
N12—C11—H11B	109.3	C31—C32—H32B	109.5
N11—C11—H11B	109.3	H32A—C32—H32B	109.5
H11A—C11—H11B	107.9	C31—C32—H32C	109.5
N13—C12—N12	111.64 (10)	H32A—C32—H32C	109.5
N13—C12—H12A	109.3	H32B—C32—H32C	109.5
N12—C12—H12A	109.3	C41—O41—Co1	128.97 (8)
N13—C12—H12B	109.3	C41—O41—H41	109.5
N12—C12—H12B	109.3	Co1—O41—H41	121.3
H12A—C12—H12B	108.0	O41—C41—C42	112.33 (13)
N14—C13—N13	112.16 (10)	O41—C41—H41A	109.1
N14—C13—H13A	109.2	C42—C41—H41A	109.1
N13—C13—H13A	109.2	O41—C41—H41B	109.1
N14—C13—H13B	109.2	C42—C41—H41B	109.1
N13—C13—H13B	109.2	H41A—C41—H41B	107.9
H13A—C13—H13B	107.9	C41—C42—H42A	109.5
N14—C14—N11	112.31 (10)	C41—C42—H42B	109.5
N14—C14—H14A	109.1	H42A—C42—H42B	109.5
N11—C14—H14A	109.1	C41—C42—H42C	109.5
N14—C14—H14B	109.1	H42A—C42—H42C	109.5
N11—C14—H14B	109.1	H42B—C42—H42C	109.5
H14A—C14—H14B	107.9		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···S2^{i}	0.99	2.87	3.6586 (13)	137
C12—H12*B*···S1^{ii}	0.99	2.92	3.8813 (13)	164
C15—H15*A*···S1^{iii}	0.99	2.99	3.9387 (13)	161
C15—H15*B*···S2^{iv}	0.99	2.94	3.7110 (13)	135
C16—H16*A*···O21	0.99	2.54	3.1009 (16)	116
C16—H16*B*···N1	0.99	2.47	3.1083 (17)	122
O21—H21···N13^{ii}	0.84	2.03	2.8424 (14)	161
C22—H22*C*···S1^{v}	0.98	3.02	3.9559 (16)	161

O31—H31···N12^{vi}	0.84	1.96	2.7969 (14)	172
O41—H41···S2^{vi}	0.84	2.37	3.2080 (10)	174

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1/2, −*y*+1/2, *z*−1/2; (iv) *x*+1/2, −*y*+1/2, *z*−1/2; (v) *x*−1, *y*, *z*; (vi) *x*+1/2, −*y*+1/2, *z*+1/2.