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Crystal structures of (acetonitrile-κ*N*)tris(pyridine-4-thioamide-κ*N*)bis(thiocyanato-κ*N*)cobalt(II) acetonitrile disolvate and tetrakis(pyridine-4-thioamide-κ*N*)bis(thiocyanato-κ*N*)nickel(II) methanol pentasolvate

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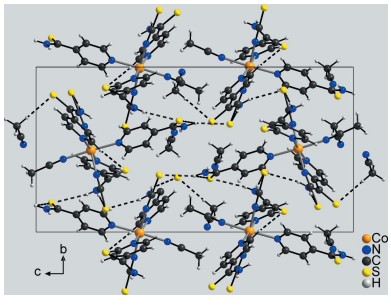
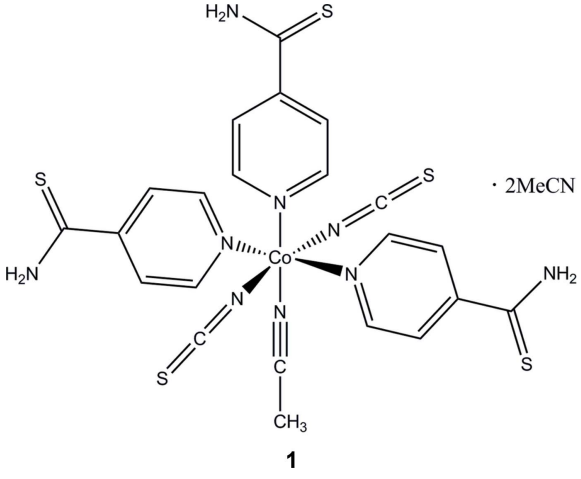
Reaction of $Co(NCS)_2$ or $Ni(NCS)_2$ with pyridine-4-thioamide in different solvents led to the formation of two compounds with composition $[Co(NCS)_2(C_2H_3N)(C_6H_6N_2S)_3]\cdot 2CH_3CN$ (**1**) and $[Ni(NCS)_2(C_6H_6N_2S)_4]\cdot 5CH_3OH$ (**2**), respectively. The asymmetric unit of compound **1** consists of one cobalt(II) cation, two thiocyanate anions, three pyridine-4-thioamide ligands, one coordinating and two solvate acetonitrile molecules. One of the two acetonitrile solvate molecules is disordered over two sets of sites in a 0.62:0.38 ratio. The asymmetric unit of compound **2** comprises of one nickel(II) cation, two thiocyanate anions, four N-bonding pyridine-4-thioamide ligands and five methanol solvate molecules. In compound **1**, the cobalt(II) cations are octahedrally coordinated into discrete complexes by two terminal N-bonding thiocyanate anions, the N atoms of three pyridine-4-thioamide ligands and one acetonitrile molecule. Additional acetonitrile solvate molecules are located between the complexes,. The complexes and solvate molecules are linked *via* intermolecular hydrogen bonding into a three-dimensional framework. In compound **2**, the nickel(II) cations are likewise octahedrally coordinated by two terminal N-bonded thiocyanate anions and four N-bonding pyridine-4-thioamide ligands into discrete complexes. From their arrangement cavities are formed, in which the methanol solvate molecules are located. Again, the complexes and solvate molecules are linked into a three-dimensional framework by intermolecular hydrogen bonding.

1. Chemical context

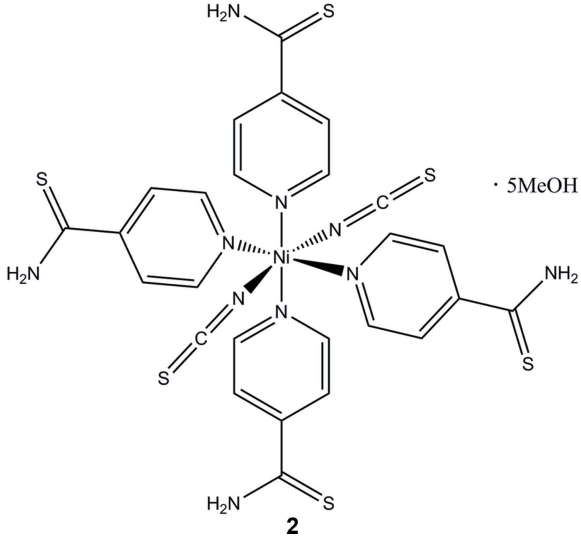
For several years we have been interested in the structural, thermal and magnetic properties of coordination compounds and polymers based on transition metal thio- and seleno-cyanates (Wöhlert *et al.*, 2013*a*, 2014*a*). In contrast to other three-atomic ligands such as, for example azides, these ligands show a more versatile coordination behaviour, including a terminal coordination and a number of different bridging modes. Therefore they are of interest from a structural point of view (Massoud *et al.*, 2013; Mousavi *et al.*, 2012; Prananto *et al.*, 2017; Kabešová *et al.*, 1995; Palion-Gazda *et al.*, 2017). Moreover, if paramagnetic metal cations are linked by these anionic ligands into chains or layers, cooperative magnetic phenomena can be expected. Hence the rational synthesis of such compounds is in the focus of our investigations (Palion-Gazda *et al.*, 2015; Wöhlert *et al.*, 2013*a*). In this context, compounds of special interest include those in which the metal



cations are linked by pairs of anionic ligands into linear chains because they can exhibit one-dimensional or three-dimensional ferromagnetic ordering, as shown recently for a number of compounds derived from $Co(NCS)_2$ (Rams *et al.*, 2017*a*,*b*; Wöhlert *et al.* 2012, 2013*b*, 2014*b*; Werner *et al.*, 2015). Unfortunately, the paramagnetic metal cations Co^{II} or Ni^{II} are less chalcophilic and therefore do not form compounds with polymeric structures from solutions, but with discrete complexes instead. In the majority of cases, these cations are octahedrally coordinated by two anionic ligands and four monodentate N-donor co-ligands. However, if such complexes are heated, they frequently decompose in discrete steps, forming new compounds as intermediates in which the metal cations are linked into one- or two-dimensional network structures. This is the reason why we are also interested in such simple complexes or their solvates (Suckert *et al.*, 2017).



1



2

In the course of our project we became interested in the monodentate ligand pyridine-4-thioamide, which might be able to link $M(NCS)_2$ chains (M = Co, Ni) into layers by intermolecular N—H···S hydrogen bonding. For example, this motif is observed in the crystal structure of the pure ligand (Colleter & Gadret, 1967; Eccles *et al.*, 2014). Moreover, one compound derived from $Cd(NCS)_2$ is known in which the

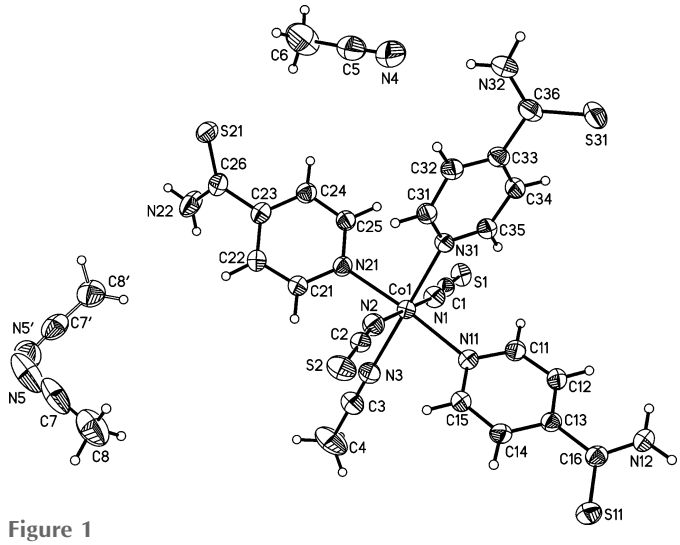


Figure 1
View of the asymmetric unit of compound **1** with atom labelling and displacement ellipsoids drawn at the 50% probability level. The disordered acetonitrile solvent molecule is shown with both orientations.

metal cations are linked by pairs of anionic ligands into chains (Neumann *et al.*, 2016). Therefore we attempted in the synthesis of discrete precursor complexes or solvates in which the anionic ligands are only terminal N-bonding to transform them subsequently into the desired chain compounds by thermal annealing. Unfortunately, no pure samples could be obtained (Neumann *et al.*, 2017,2018). In the course of this work we obtained two additional compounds from acetonitrile or methanol solution, *viz*. $[Co(NCS)_2(C_6H_6N_2S)_3(C_2H_3N)]\cdot 2C_2H_3N$ (**1**) and $[Ni(NCS)_2(C_6H_6N_2S)_4]\cdot 5CH_3OH$ (**2**), for which the CN stretching vibration is observed at 2081 cm^{-1} (**1**) and 2101 cm^{-1} (**2**), respectively. As a consequence, their

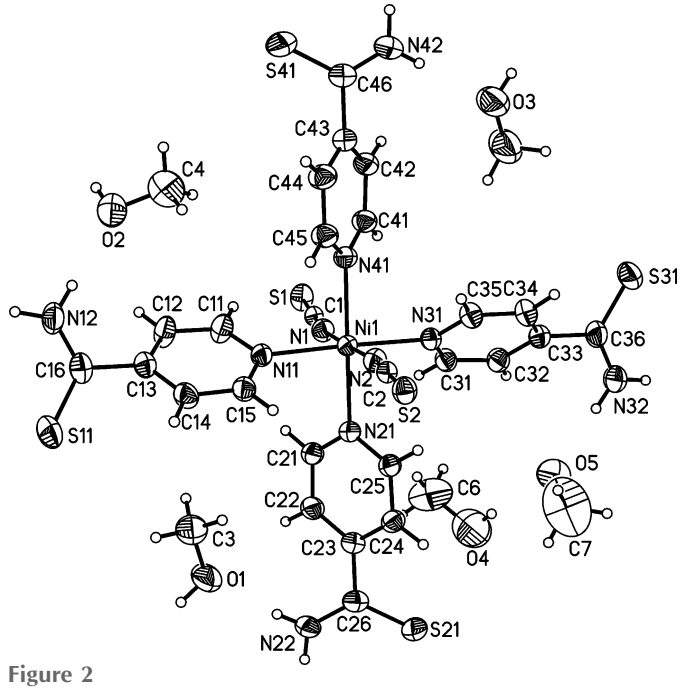


Figure 2
View of the asymmetric unit of compound **2** with atom labelling and displacement ellipsoids drawn at the 50% probability level.

Table 1
Selected geometric parameters (Å, °) for **1**.

Co1—N1	2.0650 (16)	Co1—N31	2.1785 (14)
Co1—N2	2.0720 (16)	Co1—N3	2.1950 (15)
Co1—N21	2.1666 (15)	Co1—N11	2.2032 (15)
N1—Co1—N2	177.65 (6)	N21—Co1—N3	88.82 (6)
N1—Co1—N21	91.08 (6)	N31—Co1—N3	177.72 (6)
N2—Co1—N21	88.02 (6)	N1—Co1—N11	92.70 (6)
N1—Co1—N31	89.52 (6)	N2—Co1—N11	88.06 (6)
N2—Co1—N31	92.66 (6)	N21—Co1—N11	174.69 (5)
N21—Co1—N31	90.26 (6)	N31—Co1—N11	93.50 (5)
N1—Co1—N3	88.41 (6)	N3—Co1—N11	87.56 (6)
N2—Co1—N3	89.39 (6)		

Table 2
Selected geometric parameters (Å, °) for **2**.

Ni1—N1	2.0435 (18)	Ni1—N31	2.1250 (17)
Ni1—N2	2.0526 (18)	Ni1—N41	2.1262 (17)
Ni1—N21	2.1157 (16)	Ni1—N11	2.1316 (17)
N1—Ni1—N2	178.69 (7)	N21—Ni1—N41	179.30 (7)
N1—Ni1—N21	90.21 (7)	N31—Ni1—N41	90.22 (7)
N2—Ni1—N21	90.67 (7)	N1—Ni1—N11	91.28 (7)
N1—Ni1—N31	89.06 (7)	N2—Ni1—N11	89.71 (7)
N2—Ni1—N31	89.98 (7)	N21—Ni1—N11	88.91 (6)
N21—Ni1—N31	89.16 (6)	N31—Ni1—N11	178.04 (6)
N1—Ni1—N41	89.46 (7)	N41—Ni1—N11	91.72 (7)
N2—Ni1—N41	89.65 (7)		

structures should consist of discrete complexes with terminal N-bonded thiocyanate anions and additional solvate molecules, even if these wave numbers are at the borderline of those expected for the desired bridging anionic ligands. To check if our assumption can be verified, we have performed single-crystal structure determinations of **1** and **2** and report the results in this communication.

2. Structural commentary

Unfortunately, **1** and **2** could not be prepared as pure phases and were either contaminated with additional unknown crystalline phases or, if an excess of pyridine-4-thioamide was used, with this less soluble ligand. Therefore, no further investigations regarding physical properties were performed.

The asymmetric unit of compound **1** consists of one cobalt(II) cation, two thiocyanate anions, three pyridine-4-thioamide ligands and three acetonitrile molecules. One of the two acetonitrile solvate molecules is disordered over two sets of sites in a refined ratio of 0.62:0.38. The Co^{II} cation is octahedrally coordinated by two terminal N-bonding thiocyanate anions, an acetonitrile molecule and the pyridine N atoms of three pyridine-4-thioamide ligands into a discrete complex with the same ligand types *trans*-positioned to each other (Fig. 1). The Co—N bond lengths to the thiocyanate anions are significantly shorter than those to the pyridine N atoms (Table 1), in agreement with values for similar structures (Goodgame *et al.*, 2003; Prananto *et al.*, 2017). The bond angles deviate from ideal values, showing that the octahedra are slightly distorted (Table 1).

The asymmetric unit of compound **2** comprises of one nickel(II) cation, two thiocyanate anions, four N-bonded pyridine-4-thioamide ligands and five methanol solvate molecules (Fig. 2). The Ni^{II} cation is also octahedrally coordinated by N atoms, but in this case by four pyridine-4-thioamide ligands and two terminal thiocyanate anions. Bond lengths and angles (Table 2) are comparable to those in the structure of compound **1**, but the NiN_6 octahedron is less distorted than the CoN_6 octahedron. It is noted that in both structures the pyridine-4-thioamide ligands are not planar. The thioamide groups are rotated differently out of the pyridine ring plane, with dihedral angles in the range 5.3 (2)–54.5 (2)° for **1** and 40.7 (2)–47.2 (2)° for **2**.

3. Supramolecular features

In the crystal structure of compound **1**, the discrete complexes are linked by intermolecular N—H···S hydrogen bonding between the H atoms of the amino groups and the S atoms of the thiocyanate anions or the pyridine-4-thioamide ligands into a three-dimensional framework (Fig. 3, Table 3). The complexes are arranged in such a way that cavities are formed in which additional acetonitrile molecules are embedded. These solvate molecules are linked together *via* C—H···N interactions between the methyl H atoms and the N atom of the acetonitrile molecules, but are also connected to the metal complexes by intermolecular C—H···N and C—H···S interactions.

In the crystal structure of compound **2**, a variety of different hydrogen-bonding interactions is observed in which the methanol solvate molecules act both as acceptor and donor groups. Like in compound **1**, the complexes are connected into a three-dimensional framework by intermolecular N—H···S hydrogen bonding between the H atoms of the amino groups and the S atoms of the thiocyanate anions. Again, cavities are formed that host the methanol solvate molecules. These molecules are linked by intermolecular O—H···O hydrogen

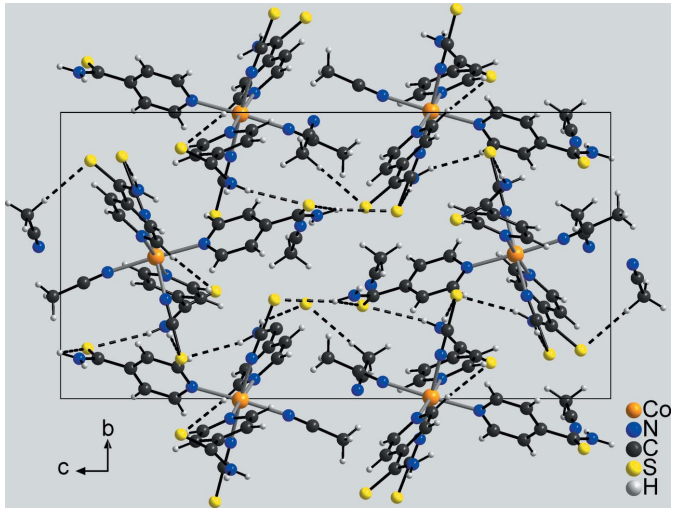


Figure 3
Crystal structure of compound **1** in a view along the *a* axis. Intermolecular hydrogen bonding is shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*C*···N5′^{i}	0.98	2.37	3.081 (12)	129
C6—H6*C*···S31^{ii}	0.98	3.02	3.901 (3)	150
C11—H11···S21^{i}	0.95	2.83	3.6556 (18)	146
C12—H12···S1^{iii}	0.95	3.01	3.8491 (18)	148
N12—H1*N*···S1^{iii}	0.88	2.66	3.5097 (17)	163
N12—H2*N*···S2^{i}	0.88	2.71	3.5731 (17)	167
C21—H21···N3	0.95	2.63	3.134 (3)	114
C22—H22···N5^{iv}	0.95	2.50	3.384 (7)	154
C25—H25···S2^{v}	0.95	2.91	3.7172 (18)	144
N22—H3*N*···S1^{vi}	0.88	2.59	3.4715 (19)	179
N22—H4*N*···S31^{v}	0.88	2.87	3.729 (2)	167
C34—H34···S11^{vii}	0.95	2.98	3.7698 (19)	142
C35—H35···N1	0.95	2.56	3.094 (2)	116
C35—H35···S21^{i}	0.95	2.95	3.7301 (19)	140
N32—H5*N*···S2^{viii}	0.88	2.74	3.5390 (18)	152
N32—H6*N*···N4	0.88	2.10	2.951 (3)	164
C8—H8*B*···S11^{vi}	0.98	2.76	3.728 (19)	172
C8′—H8*D*···N5′^{iv}	0.98	2.46	3.26 (2)	140
C8′—H8*F*···S11^{ix}	0.98	2.88	3.65 (3)	137

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, -y+1, -z+2$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (vi) $x-1, y, z$; (vii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (viii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ix) $-x+1, -y+1, -z+2$.

bonding to other methanol molecules, but are also connected to the complexes by N—H···O and O—H···S hydrogen bonds to the amino groups and the S atoms of the pyridine-4-thioamide ligands and to the thiocyanate S atoms (Fig. 4, Table 4). Finally, C—H···N and C—H···S interactions consolidate the packing of the molecules in the structure.

4. Database survey

There are only two cobalt thiocyanate derivatives with additional pyridine-4-thioamide ligands reported in the Cambridge Structure Database (Version 5.39, last update February 2018; Groom *et al.*, 2016). In tetrakis(pyridine-4-carbothioamide-κN^1)bis-(thiocyanato-κN)cobalt(II) methanol monosolvate and tetrakis(pyridine-4-carbothioamide-κN^1)bis-(thiocyanato-κN)cobalt(II) monohydrate, the Co^{II} cations are octahedrally coordinated by four pyridine-4-carbothioamide ligands and two thiocyanate anions, with the different types of solvent molecules being located in cavities of the structure (Neumann *et al.*, 2017, 2018). In $Zn(NCS)_2$(pyridine-4-thioamide)$_2$, the Zn^{II} cations are tetrahedrally coordinated by two thiocyanate anions and two pyridine-4-thioamide ligands (Neumann *et al.*, 2018). In addition there is one compound with cadmium, in which the Cd^{II} cations are octahedrally coordinated by two terminal N-bonded pyridinethioamide ligands and four thiocyanate anions and linked by pairs of anionic ligands into linear chains (Neumann *et al.*, 2016). Alongside the structure of the pure pyridine-4-thioamide ligand (Colleter & Gadret, 1967; Eccles *et al.*, 2014), its protonated form with iodide as counter-anion was reported by Shotonwa & Boeré (2014).

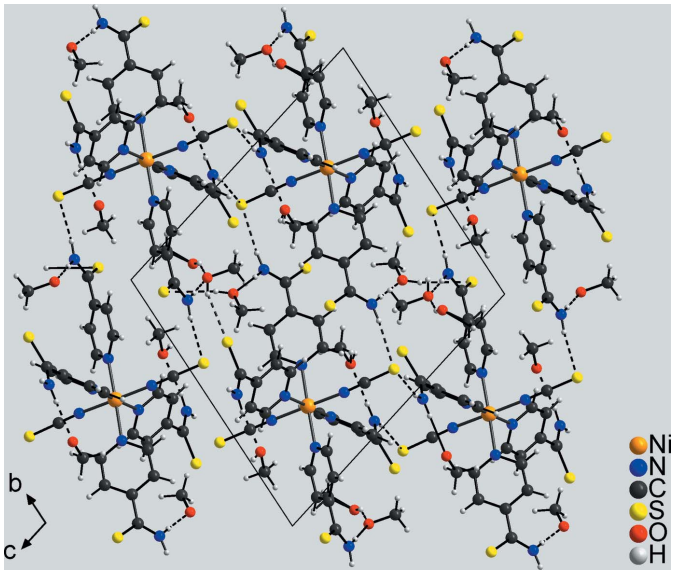


Figure 4
Crystal structure of compound **2** in a view along the *a* axis. Intermolecular hydrogen bonding is shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···S2^{i}	0.84	2.88	3.409 (2)	123
O1—H1···S11^{ii}	0.84	2.92	3.578 (2)	137
O2—H2···S31^{iii}	0.84	2.62	3.413 (3)	157
O3—H3···S1^{iv}	0.84	2.77	3.427 (2)	136
O3—H3···S31^{v}	0.84	2.93	3.576 (2)	135
C5—H5*A*···S31^{v}	0.98	3.03	3.632 (4)	121
O4—H4···O5	0.84	1.92	2.708 (5)	156
C6—H6*B*···S31^{vi}	0.98	2.73	3.566 (4)	143
O5—H5···S41^{vii}	0.84	2.51	3.216 (3)	142
C7—H7*A*···S41^{vii}	0.98	2.93	3.528 (5)	121
C11—H11···N1	0.95	2.52	3.063 (3)	117
C11—H11···S1^{viii}	0.95	2.73	3.442 (2)	133
C12—H12···S1^{viii}	0.95	2.96	3.542 (2)	121
C15—H15···N2	0.95	2.61	3.097 (3)	113
N12—H1*N*···O2	0.88	2.02	2.898 (3)	177
N12—H2*N*···S2^{ix}	0.88	2.58	3.446 (2)	171
C21—H21···N1	0.95	2.65	3.109 (3)	110
C25—H25···N2	0.95	2.66	3.122 (3)	111
C25—H25···S2^{x}	0.95	2.94	3.846 (2)	159
N22—H4*N*···S2^{xi}	0.88	2.64	3.4939 (19)	163
N22—H3*N*···O1	0.88	2.10	2.978 (3)	174
N32—H5*N*···O5	0.88	1.95	2.833 (3)	180
N32—H6*N*···S1^{vi}	0.88	2.64	3.478 (2)	159
C45—H45···S11^{ix}	0.95	2.89	3.673 (2)	141
N42—H7*N*···O3	0.88	2.08	2.957 (3)	173
N42—H8*N*···S1^{xii}	0.88	2.88	3.749 (2)	169

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

5. Synthesis and crystallization

$Co(NCS)_2$ and pyridine-4-thioamide were purchased from Alfa Aesar. $Ni(NCS)_2$ was prepared by the reaction of equimolar amounts of $Ba(SCN)_2{\cdot}3H_2O$ with $NiSO_4{\cdot}6H_2O$ in water. The colourless precipitate of $BaSO_4$ was filtered off and the resulting clear solution was evaporated until complete dryness. The purity of $Ni(NCS)_2$ was checked by X-ray powder diffraction measurements.

Table 5
Experimental details.

	1	2
Crystal data		
Chemical formula	$[Co(NCS)_2(C_2H_3N)(C_6H_6N_2S)_3]\cdot 2C_2H_3N$	$[Ni(NCS)_2(C_6H_6N_2S)_4]\cdot 5CH_4O$
M_r	712.81	887.83
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
Temperature (K)	200	200
a, b, c (Å)	11.3566 (4), 12.3251 (2), 23.7557 (8)	10.4520 (3), 14.5934 (4), 15.0580 (5)
α, β, γ (°)	90, 93.273 (3), 90	101.553 (2), 97.105 (2), 106.417 (2)
V (Å^3)	3319.69 (17)	2118.43 (11)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.87	0.80
Crystal size (mm)	0.12 × 0.10 × 0.08	0.30 × 0.18 × 0.10
Data collection		
Diffractometer	Stoe IPDS2	Stoe IPDS2
Absorption correction	–	Numerical (*X-RED* and *X-SHAPE*; Stoe, 2008)
T_{min}, T_{max}	–	0.622, 0.889
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25043, 7218, 6002	30865, 9253, 7895
R_{int}	0.027	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639	0.639
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.080, 1.04	0.039, 0.109, 1.06
No. of reflections	7218	9253
No. of parameters	419	486
No. of restraints	9	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.33	0.62, −0.57

Computer programs: *X-AREA* (Stoe, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND (Brandenburg, 1990) and publCIF (Westrip, 2010).*

Crystals of compound **1** were obtained by the reaction of 8.8 mg $Co(NCS)_2$ (0.05 mmol) with 13.8 mg pyridine-4-thioamide (0.1 mmol) in 1 ml acetonitrile. The reaction mixture was left to stand at room-temperature, leading to a few crystals of the title compound suitable for single-crystal X-ray diffraction.

For the synthesis of compound **2**, 8.8 mg $Ni(NCS)_2$ (0.05 mmol) were reacted with 27.6 mg pyridine-4-thioamide (0.2 mmol) in 3.0 ml methanol. The mixture was heated to the boiling temperature of methanol and then slowly cooled down, leading to the formation of a few crystals suitable for single-crystal X-ray diffraction.

All reaction batches were contaminated with additional crystalline phases that are unknown. If an excess of pyridine-4-thioamide was used to shift the equillibria in the directions of the discrete complexes with only coordinating pyridine-4-thioamide ligands, the batches were always contaminated with this organic ligand because it is poorly soluble in the used solvents.

IR spectra of manually selected crystals are included for both compounds in the supporting information.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. The C—H hydrogen atoms were positioned with idealized geometry (C—H = 0.95–0.98 Å; methyl H atoms were allowed to rotate but not to tip) and were refined with $U_{iso}(H) = 1.2U_{eq}(C)$ (1.5 for methyl and hydroxyl H atoms) using a riding model. The N—H hydrogen atoms were located in a difference-Fourier map, their bond lengths set to ideal values (N—H = 0.88 Å) and refined with $U_{iso}(H) = 1.5U_{eq}(N)$ using a riding model. In **1**, one of the two crystallographically independent acetonitrile solvent molecules is disordered over two sets of sites and was refined using a split model with restraints [SAME in *SHELXL* (Sheldrick, 2015)], leading to a ratio of 0.62:0.38 for the two orientations (fixed at the final stage of refinement).

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supporting information

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Crystal structures of (acetonitrile-κ*N*)tris(pyridine-4-thioamide-κ*N*)bis(thiocyanate-κ*N*)cobalt(II) acetonitrile disolvate and tetrakis(pyridine-4-thioamide-κ*N*)bis(thiocyanate-κ*N*)nickel(II) methanol pentasolvate

Tristan Neumann, Inke Jess and Christian Näther

Computing details

For both structures, data collection: *X-AREA* (Stoe, 2008); cell refinement: *X-AREA* (Stoe, 2008); data reduction: *X-AREA* (Stoe, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: Diamond (Brandenburg, 1990); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(Acetonitrile-κ*N*)tris(pyridine-4-thioamide-κ*N*)bis(thiocyanato-κ*N*)cobalt(II) acetonitrile disolvate (Compound1)

Crystal data

$[Co(NCS)_2(C_2H_3N)(C_6H_6N_2S)_3]\cdot 2C_2H_3N$
M_r = 712.81
Monoclinic, $P2_1/c$
a = 11.3566 (4) Å
b = 12.3251 (2) Å
c = 23.7557 (8) Å
β = 93.273 (3)°
V = 3319.69 (17) Å^3
Z = 4
$F(000)$ = 1468
D_x = 1.426 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25043 reflections
θ = 1.7–27.0°
μ = 0.87 mm^{-1}
T = 200 K
Block, brown
0.12 × 0.10 × 0.08 mm

Data collection

STOE IPDS-2 diffractometer
ω scans
25043 measured reflections
7218 independent reflections
6002 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.0°, θ_{min} = 1.7°
h = −14→14
k = −14→15
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.080
S = 1.04
7218 reflections
419 parameters
9 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.5907P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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}	Occ. (<1)
Co1	0.62828 (2)	0.49502 (2)	0.82672 (2)	0.02661 (7)	
N1	0.70292 (15)	0.34698 (13)	0.80907 (7)	0.0359 (3)	
C1	0.73383 (16)	0.26112 (15)	0.79702 (7)	0.0307 (4)	
S1	0.77894 (5)	0.13954 (4)	0.78062 (2)	0.03821 (11)	
N2	0.55051 (14)	0.64072 (13)	0.84732 (6)	0.0343 (3)	
C2	0.52817 (15)	0.72538 (15)	0.86457 (7)	0.0295 (4)	
S2	0.49682 (5)	0.84533 (4)	0.88860 (2)	0.04202 (12)	
N3	0.61781 (15)	0.44151 (14)	0.91443 (6)	0.0387 (4)	
C3	0.61548 (19)	0.40477 (17)	0.95811 (8)	0.0409 (4)	
C4	0.6128 (3)	0.3573 (2)	1.01395 (10)	0.0704 (8)	
H4A	0.6403	0.2820	1.0128	0.106*	
H4B	0.5319	0.3589	1.0263	0.106*	
H4C	0.6644	0.3989	1.0405	0.106*	
N4	0.3375 (2)	0.6038 (3)	0.56403 (10)	0.0857 (9)	
C5	0.2523 (3)	0.5621 (2)	0.57241 (10)	0.0576 (6)	
C6	0.1421 (3)	0.5092 (3)	0.58145 (13)	0.0799 (10)	
H6A	0.0807	0.5639	0.5858	0.120*	
H6B	0.1505	0.4647	0.6156	0.120*	
H6C	0.1200	0.4628	0.5490	0.120*	
N5	−0.1359 (7)	0.5306 (5)	1.0399 (3)	0.087 (3)	0.62
C7	−0.0520 (6)	0.5785 (5)	1.04825 (19)	0.0699 (16)	0.62
C8	0.0562 (13)	0.6419 (14)	1.0603 (7)	0.082 (4)	0.62
H8A	0.0494	0.6828	1.0954	0.123*	0.62
H8B	0.0672	0.6925	1.0292	0.123*	0.62
H8C	0.1239	0.5928	1.0643	0.123*	0.62
N5′	−0.1549 (9)	0.4866 (8)	1.0254 (4)	0.063 (2)	0.38
C7′	−0.1247 (6)	0.4336 (6)	0.9894 (3)	0.0539 (16)	0.38
C8′	−0.0796 (19)	0.3668 (18)	0.9442 (9)	0.061 (4)	0.38
H8D	−0.0008	0.3922	0.9356	0.091*	0.38
H8E	−0.1328	0.3726	0.9104	0.091*	0.38
H8F	−0.0749	0.2909	0.9564	0.091*	0.38
N11	0.80040 (13)	0.56775 (12)	0.85214 (6)	0.0302 (3)	
C11	0.89844 (17)	0.54836 (16)	0.82515 (8)	0.0339 (4)	
H11	0.8952	0.4946	0.7964	0.041*	
C12	1.00400 (17)	0.60162 (16)	0.83647 (7)	0.0340 (4)	
H12	1.0706	0.5846	0.8157	0.041*	
C13	1.01251 (16)	0.68036 (15)	0.87846 (7)	0.0293 (3)	
C14	0.91243 (17)	0.69721 (16)	0.90835 (7)	0.0333 (4)	
H14	0.9146	0.7476	0.9387	0.040*	

C15	0.80988 (17)	0.64104 (16)	0.89414 (7)	0.0332 (4)
H15	0.7426	0.6548	0.9150	0.040*
C16	1.12262 (16)	0.74442 (15)	0.89216 (7)	0.0324 (4)
N12	1.21164 (14)	0.72915 (15)	0.85928 (7)	0.0397 (4)
H1N	1.2027	0.6957	0.8266	0.060*
H2N	1.2754	0.7687	0.8661	0.060*
S11	1.13309 (5)	0.83113 (5)	0.94560 (2)	0.04363 (13)
N21	0.45275 (13)	0.43047 (12)	0.80859 (6)	0.0304 (3)
C21	0.37190 (16)	0.43714 (17)	0.84752 (8)	0.0365 (4)
H21	0.3943	0.4691	0.8829	0.044*
C22	0.25792 (17)	0.39979 (17)	0.83859 (8)	0.0378 (4)
H22	0.2043	0.4034	0.8678	0.045*
C23	0.22269 (16)	0.35688 (15)	0.78638 (8)	0.0329 (4)
C24	0.30512 (17)	0.35158 (16)	0.74560 (8)	0.0341 (4)
H24	0.2837	0.3240	0.7091	0.041*
C25	0.41881 (16)	0.38689 (15)	0.75876 (7)	0.0317 (4)
H25	0.4755	0.3799	0.7311	0.038*
C26	0.09837 (16)	0.32242 (16)	0.77362 (8)	0.0362 (4)
N22	0.05589 (16)	0.25230 (17)	0.80962 (9)	0.0536 (5)
H3N	−0.0138	0.2228	0.8021	0.080*
H4N	0.0964	0.2277	0.8396	0.080*
S21	0.02293 (4)	0.37470 (4)	0.71886 (2)	0.03954 (12)
N31	0.63857 (13)	0.54138 (12)	0.73865 (6)	0.0284 (3)
C31	0.56230 (16)	0.61090 (15)	0.71318 (7)	0.0304 (4)
H31	0.5006	0.6392	0.7342	0.037*
C32	0.56864 (17)	0.64377 (15)	0.65764 (7)	0.0329 (4)
H32	0.5107	0.6910	0.6407	0.039*
C33	0.66128 (17)	0.60637 (15)	0.62729 (7)	0.0325 (4)
C34	0.73991 (17)	0.53387 (16)	0.65314 (7)	0.0334 (4)
H34	0.8040	0.5065	0.6334	0.040*
C35	0.72442 (16)	0.50179 (15)	0.70767 (7)	0.0324 (4)
H35	0.7768	0.4492	0.7243	0.039*
C36	0.67792 (19)	0.64037 (17)	0.56790 (8)	0.0399 (4)
N32	0.58298 (19)	0.63969 (19)	0.53393 (7)	0.0565 (5)
H5N	0.5843	0.6602	0.4985	0.085*
H6N	0.5141	0.6151	0.5435	0.085*
S31	0.81118 (6)	0.67528 (6)	0.54887 (2)	0.05599 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02609 (12)	0.02759 (12)	0.02615 (11)	−0.00033 (9)	0.00155 (8)	−0.00024 (9)
N1	0.0378 (9)	0.0323 (8)	0.0376 (8)	0.0035 (7)	0.0024 (6)	0.0008 (6)
C1	0.0272 (8)	0.0343 (10)	0.0306 (8)	−0.0027 (7)	0.0019 (6)	0.0036 (7)
S1	0.0420 (3)	0.0280 (2)	0.0453 (2)	0.0007 (2)	0.0089 (2)	−0.00051 (19)
N2	0.0336 (8)	0.0337 (8)	0.0356 (7)	0.0017 (7)	0.0027 (6)	−0.0023 (6)
C2	0.0281 (9)	0.0343 (10)	0.0260 (7)	−0.0013 (7)	0.0008 (6)	0.0017 (7)
S2	0.0581 (3)	0.0324 (2)	0.0357 (2)	0.0065 (2)	0.0041 (2)	−0.00340 (19)

N3	0.0387 (9)	0.0450 (10)	0.0323 (8)	−0.0007 (8)	0.0018 (6)	0.0051 (7)
C3	0.0459 (11)	0.0408 (11)	0.0365 (10)	0.0055 (9)	0.0063 (8)	0.0020 (8)
C4	0.106 (2)	0.0678 (17)	0.0391 (11)	0.0193 (16)	0.0174 (13)	0.0178 (12)
N4	0.0587 (15)	0.141 (3)	0.0563 (13)	−0.0153 (16)	−0.0072 (11)	0.0269 (15)
C5	0.0606 (16)	0.0687 (17)	0.0430 (12)	−0.0035 (13)	−0.0019 (11)	0.0062 (11)
C6	0.099 (2)	0.081 (2)	0.0614 (16)	−0.0387 (19)	0.0166 (16)	−0.0124 (14)
N5	0.129 (7)	0.067 (4)	0.072 (4)	0.025 (4)	0.055 (4)	0.004 (3)
C7	0.101 (4)	0.062 (3)	0.051 (2)	0.038 (3)	0.041 (3)	0.021 (2)
C8	0.103 (9)	0.084 (6)	0.061 (4)	0.041 (6)	0.026 (5)	0.020 (4)
N5′	0.061 (4)	0.070 (7)	0.059 (5)	0.013 (4)	0.006 (4)	0.004 (4)
C7′	0.044 (3)	0.061 (4)	0.054 (4)	−0.002 (3)	−0.010 (3)	0.026 (3)
C8′	0.061 (7)	0.064 (8)	0.057 (9)	0.006 (7)	−0.003 (6)	0.016 (5)
N11	0.0289 (7)	0.0315 (8)	0.0300 (7)	−0.0015 (6)	0.0009 (6)	−0.0007 (6)
C11	0.0320 (9)	0.0357 (10)	0.0342 (9)	−0.0019 (8)	0.0031 (7)	−0.0070 (7)
C12	0.0300 (9)	0.0388 (10)	0.0335 (9)	−0.0020 (8)	0.0047 (7)	−0.0044 (7)
C13	0.0301 (9)	0.0312 (9)	0.0264 (8)	−0.0012 (7)	−0.0012 (6)	0.0033 (6)
C14	0.0342 (9)	0.0360 (10)	0.0296 (8)	−0.0003 (8)	0.0004 (7)	−0.0056 (7)
C15	0.0302 (9)	0.0392 (10)	0.0304 (8)	−0.0014 (8)	0.0035 (7)	−0.0039 (7)
C16	0.0333 (9)	0.0330 (9)	0.0304 (8)	−0.0019 (8)	−0.0027 (7)	0.0054 (7)
N12	0.0305 (8)	0.0489 (10)	0.0397 (8)	−0.0079 (7)	0.0009 (6)	−0.0052 (7)
S11	0.0460 (3)	0.0464 (3)	0.0382 (2)	−0.0120 (2)	0.0000 (2)	−0.0079 (2)
N21	0.0278 (7)	0.0309 (8)	0.0325 (7)	−0.0026 (6)	0.0015 (6)	−0.0017 (6)
C21	0.0308 (9)	0.0469 (11)	0.0319 (9)	−0.0028 (8)	0.0026 (7)	−0.0053 (8)
C22	0.0297 (9)	0.0481 (11)	0.0359 (9)	−0.0017 (8)	0.0046 (7)	−0.0020 (8)
C23	0.0292 (9)	0.0297 (9)	0.0395 (9)	−0.0006 (7)	−0.0004 (7)	0.0018 (7)
C24	0.0325 (9)	0.0348 (10)	0.0349 (9)	−0.0010 (8)	0.0008 (7)	−0.0032 (7)
C25	0.0307 (9)	0.0331 (9)	0.0315 (8)	−0.0023 (7)	0.0029 (7)	−0.0026 (7)
C26	0.0289 (9)	0.0351 (10)	0.0446 (10)	0.0002 (8)	0.0019 (7)	−0.0040 (8)
N22	0.0319 (9)	0.0620 (13)	0.0661 (12)	−0.0109 (9)	−0.0058 (8)	0.0201 (10)
S21	0.0325 (2)	0.0461 (3)	0.0393 (2)	0.0015 (2)	−0.00403 (18)	−0.0051 (2)
N31	0.0294 (7)	0.0308 (7)	0.0253 (6)	−0.0011 (6)	0.0026 (5)	0.0001 (5)
C31	0.0299 (9)	0.0317 (9)	0.0298 (8)	0.0007 (7)	0.0027 (7)	0.0004 (7)
C32	0.0344 (9)	0.0327 (9)	0.0313 (8)	0.0004 (8)	−0.0005 (7)	0.0017 (7)
C33	0.0373 (10)	0.0324 (9)	0.0279 (8)	−0.0075 (8)	0.0011 (7)	−0.0014 (7)
C34	0.0327 (9)	0.0382 (10)	0.0299 (8)	−0.0014 (8)	0.0051 (7)	−0.0032 (7)
C35	0.0305 (9)	0.0363 (10)	0.0304 (8)	0.0017 (8)	0.0024 (7)	−0.0001 (7)
C36	0.0496 (12)	0.0416 (11)	0.0288 (8)	−0.0045 (9)	0.0054 (8)	0.0012 (8)
N32	0.0536 (12)	0.0857 (15)	0.0298 (8)	−0.0040 (11)	−0.0003 (8)	0.0136 (9)
S31	0.0562 (3)	0.0740 (4)	0.0391 (3)	−0.0196 (3)	0.0143 (2)	0.0030 (3)

Geometric parameters (Å, º)

Co1—N1	2.0650 (16)	C14—C15	1.380 (3)
Co1—N2	2.0720 (16)	C14—H14	0.9500
Co1—N21	2.1666 (15)	C15—H15	0.9500
Co1—N31	2.1785 (14)	C16—N12	1.326 (2)
Co1—N3	2.1950 (15)	C16—S11	1.6583 (19)
Co1—N11	2.2032 (15)	N12—H1N	0.8799

N1—C1	1.156 (2)	N12—H2N	0.8800
C1—S1	1.6378 (19)	N21—C25	1.336 (2)
N2—C2	1.155 (2)	N21—C21	1.342 (2)
C2—S2	1.6314 (19)	C21—C22	1.379 (3)
N3—C3	1.134 (2)	C21—H21	0.9500
C3—C4	1.451 (3)	C22—C23	1.386 (3)
C4—H4A	0.9800	C22—H22	0.9500
C4—H4B	0.9800	C23—C24	1.387 (3)
C4—H4C	0.9800	C23—C26	1.489 (3)
N4—C5	1.123 (4)	C24—C25	1.381 (3)
C5—C6	1.439 (4)	C24—H24	0.9500
C6—H6A	0.9800	C25—H25	0.9500
C6—H6B	0.9800	C26—N22	1.326 (3)
C6—H6C	0.9800	C26—S21	1.647 (2)
N5—C7	1.129 (8)	N22—H3N	0.8799
C7—C8	1.470 (14)	N22—H4N	0.8800
C8—H8A	0.9800	N31—C31	1.338 (2)
C8—H8B	0.9800	N31—C35	1.346 (2)
C8—H8C	0.9800	C31—C32	1.386 (2)
N5′—C7′	1.144 (9)	C31—H31	0.9500
C7′—C8′	1.469 (15)	C32—C33	1.388 (3)
C8′—H8D	0.9800	C32—H32	0.9500
C8′—H8E	0.9800	C33—C34	1.382 (3)
C8′—H8F	0.9800	C33—C36	1.494 (2)
N11—C11	1.338 (2)	C34—C35	1.375 (2)
N11—C15	1.346 (2)	C34—H34	0.9500
C11—C12	1.380 (3)	C35—H35	0.9500
C11—H11	0.9500	C36—N32	1.309 (3)
C12—C13	1.391 (3)	C36—S31	1.661 (2)
C12—H12	0.9500	N32—H5N	0.8800
C13—C14	1.390 (2)	N32—H6N	0.8799
C13—C16	1.499 (3)		

N1—Co1—N2	177.65 (6)	C15—C14—C13	120.22 (16)
N1—Co1—N21	91.08 (6)	C15—C14—H14	119.9
N2—Co1—N21	88.02 (6)	C13—C14—H14	119.9
N1—Co1—N31	89.52 (6)	N11—C15—C14	123.29 (16)
N2—Co1—N31	92.66 (6)	N11—C15—H15	118.4
N21—Co1—N31	90.26 (6)	C14—C15—H15	118.4
N1—Co1—N3	88.41 (6)	N12—C16—C13	116.87 (16)
N2—Co1—N3	89.39 (6)	N12—C16—S11	121.24 (15)
N21—Co1—N3	88.82 (6)	C13—C16—S11	121.88 (13)
N31—Co1—N3	177.72 (6)	C16—N12—H1N	122.2
N1—Co1—N11	92.70 (6)	C16—N12—H2N	117.4
N2—Co1—N11	88.06 (6)	H1N—N12—H2N	118.3
N21—Co1—N11	174.69 (5)	C25—N21—C21	117.44 (16)
N31—Co1—N11	93.50 (5)	C25—N21—Co1	122.63 (12)
N3—Co1—N11	87.56 (6)	C21—N21—Co1	119.88 (12)

C1—N1—Co1	173.25 (16)	N21—C21—C22	123.13 (17)
N1—C1—S1	179.26 (19)	N21—C21—H21	118.4
C2—N2—Co1	166.49 (16)	C22—C21—H21	118.4
N2—C2—S2	179.66 (17)	C21—C22—C23	119.05 (17)
C3—N3—Co1	173.73 (17)	C21—C22—H22	120.5
N3—C3—C4	179.7 (3)	C23—C22—H22	120.5
C3—C4—H4A	109.5	C22—C23—C24	118.11 (17)
C3—C4—H4B	109.5	C22—C23—C26	120.86 (16)
H4A—C4—H4B	109.5	C24—C23—C26	120.96 (16)
C3—C4—H4C	109.5	C25—C24—C23	119.13 (17)
H4A—C4—H4C	109.5	C25—C24—H24	120.4
H4B—C4—H4C	109.5	C23—C24—H24	120.4
N4—C5—C6	178.3 (3)	N21—C25—C24	123.06 (16)
C5—C6—H6A	109.5	N21—C25—H25	118.5
C5—C6—H6B	109.5	C24—C25—H25	118.5
H6A—C6—H6B	109.5	N22—C26—C23	115.48 (17)
C5—C6—H6C	109.5	N22—C26—S21	124.91 (16)
H6A—C6—H6C	109.5	C23—C26—S21	119.58 (14)
H6B—C6—H6C	109.5	C26—N22—H3N	119.6
N5—C7—C8	178.7 (8)	C26—N22—H4N	123.7
C7—C8—H8A	109.5	H3N—N22—H4N	116.4
C7—C8—H8B	109.5	C31—N31—C35	117.08 (14)
H8A—C8—H8B	109.5	C31—N31—Co1	122.23 (11)
C7—C8—H8C	109.5	C35—N31—Co1	120.68 (12)
H8A—C8—H8C	109.5	N31—C31—C32	123.38 (16)
H8B—C8—H8C	109.5	N31—C31—H31	118.3
N5′—C7′—C8′	177.0 (11)	C32—C31—H31	118.3
C7′—C8′—H8D	109.5	C31—C32—C33	118.66 (17)
C7′—C8′—H8E	109.5	C31—C32—H32	120.7
H8D—C8′—H8E	109.5	C33—C32—H32	120.7
C7′—C8′—H8F	109.5	C34—C33—C32	118.28 (16)
H8D—C8′—H8F	109.5	C34—C33—C36	119.17 (17)
H8E—C8′—H8F	109.5	C32—C33—C36	122.54 (18)
C11—N11—C15	116.21 (16)	C35—C34—C33	119.35 (17)
C11—N11—Co1	123.08 (12)	C35—C34—H34	120.3
C15—N11—Co1	120.56 (12)	C33—C34—H34	120.3
N11—C11—C12	124.01 (17)	N31—C35—C34	123.11 (17)
N11—C11—H11	118.0	N31—C35—H35	118.4
C12—C11—H11	118.0	C34—C35—H35	118.4
C11—C12—C13	119.72 (17)	N32—C36—C33	115.85 (18)
C11—C12—H12	120.1	N32—C36—S31	124.40 (15)
C13—C12—H12	120.1	C33—C36—S31	119.75 (15)
C14—C13—C12	116.44 (17)	C36—N32—H5N	121.9
C14—C13—C16	120.45 (16)	C36—N32—H6N	123.8
C12—C13—C16	123.11 (16)	H5N—N32—H6N	114.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*C*···N5′^{i}	0.98	2.37	3.081 (12)	129
C6—H6*C*···S31^{ii}	0.98	3.02	3.901 (3)	150
C11—H11···S21^{i}	0.95	2.83	3.6556 (18)	146
C12—H12···S1^{iii}	0.95	3.01	3.8491 (18)	148
N12—H1*N*···S1^{iii}	0.88	2.66	3.5097 (17)	163
N12—H2*N*···S2^{i}	0.88	2.71	3.5731 (17)	167
C21—H21···N3	0.95	2.63	3.134 (3)	114
C22—H22···N5^{iv}	0.95	2.50	3.384 (7)	154
C25—H25···S2^{v}	0.95	2.91	3.7172 (18)	144
N22—H3*N*···S1^{vi}	0.88	2.59	3.4715 (19)	179
N22—H4*N*···S31^{v}	0.88	2.87	3.729 (2)	167
C34—H34···S11^{vii}	0.95	2.98	3.7698 (19)	142
C35—H35···N1	0.95	2.56	3.094 (2)	116
C35—H35···S21^{i}	0.95	2.95	3.7301 (19)	140
N32—H5*N*···S2^{viii}	0.88	2.74	3.5390 (18)	152
N32—H6*N*···N4	0.88	2.10	2.951 (3)	164
C8—H8*B*···S11^{vi}	0.98	2.76	3.728 (19)	172
C8′—H8*D*···N5′^{iv}	0.98	2.46	3.26 (2)	140
C8′—H8*F*···S11^{ix}	0.98	2.88	3.65 (3)	137

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+2, *y*+1/2, −*z*+3/2; (iv) −*x*, −*y*+1, −*z*+2; (v) −*x*+1, *y*−1/2, −*z*+3/2; (vi) *x*−1, *y*, *z*; (vii) −*x*+2, *y*−1/2, −*z*+3/2; (viii) *x*, −*y*+3/2, *z*−1/2; (ix) −*x*+1, −*y*+1, −*z*+2.

Tetrakis(pyridine-4-thioamide-κ*N*)bis(thiocyanato-κ*N*)nickel(II) methanol pentasolvate (Compound2)

Crystal data

$[Ni(NCS)_2(C_6H_6N_2S)_4]\cdot 5CH_4O$
M_r = 887.83
Triclinic, $P\overline{1}$
a = 10.4520 (3) Å
b = 14.5934 (4) Å
c = 15.0580 (5) Å
α = 101.553 (2)°
β = 97.105 (2)°
γ = 106.417 (2)°
V = 2118.43 (11) Å^3
Z = 2
F(000) = 928
D_x = 1.392 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 30865 reflections
θ = 1.5–27.0°
μ = 0.80 mm^{-1}
T = 200 K
Block, yellow
0.30 × 0.18 × 0.10 mm

Data collection

STOE IPDS-2 diffractometer
ω scans
Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)
T_{min} = 0.622, T_{max} = 0.889
30865 measured reflections
9253 independent reflections
7895 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.0°, θ_{min} = 1.5°
h = −13→13
k = −18→18
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109

S = 1.06
9253 reflections
486 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 1.0537P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.026$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}

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}
Ni1	0.51341 (2)	0.75649 (2)	0.25835 (2)	0.02541 (8)
N1	0.54979 (18)	0.69614 (13)	0.13314 (13)	0.0327 (4)
C1	0.55335 (19)	0.66218 (14)	0.05750 (14)	0.0274 (4)
S1	0.55930 (7)	0.61468 (4)	−0.04898 (4)	0.03984 (14)
N2	0.47316 (17)	0.81774 (12)	0.38258 (12)	0.0312 (4)
C2	0.45784 (19)	0.84815 (14)	0.45634 (14)	0.0270 (4)
S2	0.43803 (5)	0.89172 (4)	0.56086 (4)	0.03231 (12)
O1	1.11056 (19)	0.76700 (17)	0.45151 (19)	0.0685 (6)
H1	1.1714	0.7529	0.4827	0.103*
C3	0.9826 (3)	0.7028 (2)	0.4528 (3)	0.0619 (8)
H3A	0.9932	0.6612	0.4951	0.093*
H3B	0.9412	0.6610	0.3905	0.093*
H3C	0.9240	0.7413	0.4737	0.093*
O2	0.2866 (3)	0.29719 (16)	0.25572 (19)	0.0746 (7)
H2	0.2560	0.2466	0.2117	0.112*
C4	0.2076 (4)	0.3592 (3)	0.2485 (3)	0.0869 (11)
H4A	0.2268	0.4087	0.3071	0.130*
H4B	0.1111	0.3202	0.2341	0.130*
H4C	0.2294	0.3923	0.1991	0.130*
O3	−0.1063 (2)	0.74182 (19)	0.0459 (2)	0.0769 (7)
H3	−0.1766	0.7415	0.0120	0.115*
C5	0.0077 (4)	0.7993 (3)	0.0215 (4)	0.0954 (14)
H5A	−0.0007	0.8647	0.0224	0.143*
H5B	0.0151	0.7679	−0.0407	0.143*
H5C	0.0891	0.8060	0.0655	0.143*
O4	0.9917 (4)	1.1226 (3)	0.1994 (3)	0.1172 (11)
H4	0.9255	1.1374	0.2174	0.176*
C6	0.9483 (5)	1.0242 (3)	0.1498 (3)	0.0990 (14)
H6A	1.0269	1.0004	0.1471	0.149*
H6B	0.9032	1.0186	0.0869	0.149*
H6C	0.8843	0.9844	0.1804	0.149*
O5	0.7792 (3)	1.1926 (2)	0.2133 (2)	0.0917 (9)
H5	0.8183	1.2328	0.1847	0.138*

C7	0.8085 (7)	1.2391 (5)	0.3032 (4)	0.138 (2)
H7A	0.8012	1.3054	0.3079	0.208*
H7B	0.9017	1.2459	0.3307	0.208*
H7C	0.7455	1.2058	0.3385	0.208*
N11	0.55562 (17)	0.64292 (12)	0.31467 (12)	0.0292 (3)
C11	0.5353 (3)	0.55466 (16)	0.25963 (16)	0.0399 (5)
H11	0.5032	0.5446	0.1955	0.048*
C12	0.5581 (3)	0.47683 (17)	0.29056 (16)	0.0428 (5)
H12	0.5421	0.4151	0.2483	0.051*
C13	0.6048 (2)	0.48958 (16)	0.38378 (15)	0.0336 (4)
C14	0.6301 (2)	0.58205 (16)	0.44148 (15)	0.0355 (5)
H14	0.6653	0.5947	0.5055	0.043*
C15	0.6037 (2)	0.65570 (16)	0.40479 (15)	0.0340 (4)
H15	0.6202	0.7185	0.4452	0.041*
C16	0.6263 (3)	0.40563 (17)	0.41981 (16)	0.0398 (5)
N12	0.5319 (2)	0.31979 (15)	0.38285 (15)	0.0457 (5)
H1N	0.4568	0.3147	0.3458	0.069*
H2N	0.5292	0.2622	0.3934	0.069*
S11	0.76130 (8)	0.42440 (6)	0.50051 (6)	0.0593 (2)
N21	0.72138 (16)	0.84055 (12)	0.30150 (12)	0.0286 (3)
C21	0.8184 (2)	0.80324 (16)	0.27672 (16)	0.0342 (4)
H21	0.7920	0.7383	0.2383	0.041*
C22	0.9556 (2)	0.85515 (16)	0.30453 (16)	0.0363 (5)
H22	1.0218	0.8256	0.2868	0.044*
C23	0.9951 (2)	0.95123 (16)	0.35878 (15)	0.0315 (4)
C24	0.8945 (2)	0.99054 (15)	0.38322 (15)	0.0329 (4)
H24	0.9178	1.0564	0.4192	0.040*
C25	0.7602 (2)	0.93304 (15)	0.35472 (15)	0.0315 (4)
H25	0.6922	0.9599	0.3735	0.038*
C26	1.1412 (2)	1.01136 (16)	0.38800 (15)	0.0344 (4)
N22	1.22398 (18)	0.96366 (15)	0.41365 (14)	0.0385 (4)
H4N	1.3129	0.9904	0.4262	0.058*
H3N	1.1961	0.9051	0.4250	0.058*
S21	1.19199 (6)	1.12876 (4)	0.38386 (5)	0.04608 (15)
N31	0.47817 (17)	0.87293 (12)	0.20441 (12)	0.0288 (3)
C31	0.5552 (2)	0.91431 (15)	0.14905 (15)	0.0324 (4)
H31	0.6224	0.8868	0.1296	0.039*
C32	0.5413 (2)	0.99481 (16)	0.11913 (16)	0.0359 (5)
H32	0.5997	1.0230	0.0814	0.043*
C33	0.4415 (2)	1.03440 (16)	0.14444 (16)	0.0345 (4)
C34	0.3592 (2)	0.99038 (17)	0.20028 (16)	0.0374 (5)
H34	0.2884	1.0144	0.2183	0.045*
C35	0.3820 (2)	0.91149 (16)	0.22892 (15)	0.0339 (4)
H35	0.3266	0.8830	0.2681	0.041*
C36	0.4190 (2)	1.11957 (17)	0.11202 (17)	0.0403 (5)
N32	0.5284 (2)	1.19414 (15)	0.11852 (18)	0.0520 (6)
H5N	0.6061	1.1934	0.1481	0.078*
H6N	0.5270	1.2440	0.0943	0.078*

S31	0.26248 (7)	1.11340 (5)	0.06808 (6)	0.0578 (2)
N41	0.30423 (17)	0.67290 (13)	0.21366 (12)	0.0310 (4)
C41	0.2366 (2)	0.66188 (16)	0.12907 (15)	0.0342 (4)
H41	0.2852	0.6901	0.0866	0.041*
C42	0.0993 (2)	0.61148 (16)	0.10008 (16)	0.0370 (5)
H42	0.0543	0.6076	0.0400	0.044*
C43	0.0283 (2)	0.56666 (16)	0.15998 (17)	0.0361 (5)
C44	0.0988 (2)	0.57619 (17)	0.24755 (17)	0.0398 (5)
H44	0.0540	0.5457	0.2902	0.048*
C45	0.2346 (2)	0.63047 (16)	0.27168 (16)	0.0363 (5)
H45	0.2812	0.6382	0.3324	0.044*
C46	−0.1192 (2)	0.50686 (18)	0.13038 (19)	0.0437 (5)
N42	−0.1973 (2)	0.54523 (17)	0.08483 (17)	0.0515 (5)
H7N	−0.1699	0.6010	0.0683	0.077*
H8N	−0.2852	0.5139	0.0721	0.077*
S41	−0.17085 (7)	0.39687 (6)	0.15227 (7)	0.0666 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02585 (13)	0.02370 (13)	0.02562 (13)	0.00738 (9)	0.00263 (9)	0.00581 (9)
N1	0.0353 (9)	0.0315 (9)	0.0308 (9)	0.0112 (7)	0.0047 (7)	0.0065 (7)
C1	0.0274 (9)	0.0241 (9)	0.0301 (10)	0.0079 (7)	0.0012 (7)	0.0087 (8)
S1	0.0564 (3)	0.0380 (3)	0.0263 (3)	0.0188 (3)	0.0059 (2)	0.0062 (2)
N2	0.0327 (9)	0.0288 (8)	0.0318 (9)	0.0103 (7)	0.0055 (7)	0.0063 (7)
C2	0.0243 (8)	0.0228 (9)	0.0337 (11)	0.0073 (7)	0.0023 (7)	0.0089 (8)
S2	0.0369 (3)	0.0324 (3)	0.0302 (3)	0.0145 (2)	0.0078 (2)	0.0076 (2)
O1	0.0363 (9)	0.0662 (13)	0.1032 (18)	0.0093 (9)	−0.0012 (10)	0.0403 (13)
C3	0.0440 (14)	0.0586 (17)	0.082 (2)	0.0114 (13)	0.0091 (14)	0.0225 (16)
O2	0.0758 (15)	0.0506 (12)	0.0884 (18)	0.0191 (11)	−0.0121 (12)	0.0152 (11)
C4	0.072 (2)	0.080 (3)	0.110 (3)	0.029 (2)	0.010 (2)	0.021 (2)
O3	0.0504 (11)	0.0750 (15)	0.109 (2)	0.0153 (11)	−0.0006 (12)	0.0485 (15)
C5	0.062 (2)	0.088 (3)	0.153 (4)	0.0253 (19)	0.014 (2)	0.070 (3)
O4	0.109 (2)	0.115 (3)	0.120 (3)	0.049 (2)	−0.005 (2)	0.008 (2)
C6	0.087 (3)	0.101 (3)	0.083 (3)	0.001 (2)	0.006 (2)	0.014 (2)
O5	0.0716 (16)	0.0709 (16)	0.119 (2)	0.0153 (13)	−0.0155 (15)	0.0239 (16)
C7	0.186 (6)	0.197 (6)	0.094 (4)	0.101 (5)	0.082 (4)	0.079 (4)
N11	0.0326 (8)	0.0260 (8)	0.0280 (8)	0.0093 (7)	0.0016 (7)	0.0069 (6)
C11	0.0605 (14)	0.0289 (10)	0.0282 (11)	0.0141 (10)	0.0019 (10)	0.0063 (8)
C12	0.0683 (16)	0.0283 (10)	0.0330 (11)	0.0187 (10)	0.0061 (11)	0.0076 (9)
C13	0.0369 (10)	0.0334 (10)	0.0347 (11)	0.0141 (8)	0.0067 (9)	0.0134 (9)
C14	0.0408 (11)	0.0382 (11)	0.0278 (10)	0.0151 (9)	0.0003 (8)	0.0087 (8)
C15	0.0387 (11)	0.0307 (10)	0.0303 (10)	0.0126 (8)	−0.0010 (8)	0.0046 (8)
C16	0.0509 (13)	0.0387 (12)	0.0380 (12)	0.0216 (10)	0.0107 (10)	0.0160 (9)
N12	0.0586 (13)	0.0343 (10)	0.0495 (12)	0.0189 (9)	0.0064 (10)	0.0182 (9)
S11	0.0673 (4)	0.0537 (4)	0.0597 (4)	0.0251 (3)	−0.0083 (3)	0.0239 (3)
N21	0.0260 (8)	0.0273 (8)	0.0307 (9)	0.0077 (6)	0.0030 (6)	0.0053 (7)
C21	0.0310 (10)	0.0297 (10)	0.0386 (11)	0.0114 (8)	0.0024 (8)	0.0009 (8)

C22	0.0291 (10)	0.0355 (11)	0.0428 (12)	0.0138 (8)	0.0054 (9)	0.0026 (9)
C23	0.0276 (9)	0.0341 (10)	0.0306 (10)	0.0084 (8)	0.0034 (8)	0.0063 (8)
C24	0.0305 (10)	0.0293 (10)	0.0354 (11)	0.0080 (8)	0.0053 (8)	0.0029 (8)
C25	0.0281 (9)	0.0289 (10)	0.0363 (11)	0.0098 (8)	0.0057 (8)	0.0042 (8)
C26	0.0286 (10)	0.0387 (11)	0.0317 (11)	0.0087 (8)	0.0053 (8)	0.0023 (9)
N22	0.0256 (8)	0.0417 (10)	0.0452 (11)	0.0101 (7)	0.0023 (7)	0.0076 (8)
S21	0.0317 (3)	0.0354 (3)	0.0643 (4)	0.0052 (2)	0.0027 (3)	0.0088 (3)
N31	0.0300 (8)	0.0277 (8)	0.0301 (9)	0.0096 (7)	0.0044 (7)	0.0106 (7)
C31	0.0306 (10)	0.0330 (10)	0.0375 (11)	0.0123 (8)	0.0091 (8)	0.0123 (9)
C32	0.0358 (10)	0.0336 (11)	0.0411 (12)	0.0100 (8)	0.0091 (9)	0.0157 (9)
C33	0.0357 (10)	0.0299 (10)	0.0372 (11)	0.0105 (8)	0.0011 (9)	0.0101 (8)
C34	0.0391 (11)	0.0384 (11)	0.0412 (12)	0.0199 (9)	0.0099 (9)	0.0116 (9)
C35	0.0352 (10)	0.0368 (11)	0.0354 (11)	0.0159 (9)	0.0104 (9)	0.0127 (9)
C36	0.0462 (12)	0.0348 (11)	0.0432 (13)	0.0171 (10)	0.0038 (10)	0.0139 (10)
N32	0.0485 (12)	0.0370 (11)	0.0726 (16)	0.0118 (9)	0.0008 (11)	0.0269 (10)
S31	0.0447 (3)	0.0499 (4)	0.0843 (5)	0.0191 (3)	−0.0010 (3)	0.0312 (4)
N41	0.0283 (8)	0.0304 (8)	0.0317 (9)	0.0061 (7)	0.0020 (7)	0.0088 (7)
C41	0.0316 (10)	0.0360 (11)	0.0325 (11)	0.0070 (8)	0.0020 (8)	0.0106 (9)
C42	0.0326 (10)	0.0377 (11)	0.0368 (11)	0.0081 (9)	−0.0022 (9)	0.0105 (9)
C43	0.0287 (10)	0.0315 (10)	0.0452 (13)	0.0075 (8)	0.0027 (9)	0.0087 (9)
C44	0.0349 (11)	0.0414 (12)	0.0410 (12)	0.0057 (9)	0.0070 (9)	0.0150 (10)
C45	0.0338 (10)	0.0383 (11)	0.0333 (11)	0.0056 (9)	0.0016 (8)	0.0129 (9)
C46	0.0311 (11)	0.0405 (12)	0.0548 (15)	0.0066 (9)	0.0026 (10)	0.0116 (11)
N42	0.0308 (10)	0.0495 (12)	0.0692 (15)	0.0080 (9)	−0.0023 (10)	0.0176 (11)
S41	0.0384 (3)	0.0507 (4)	0.1036 (7)	−0.0017 (3)	−0.0032 (4)	0.0362 (4)

Geometric parameters (Å, º)

Ni1—N1	2.0435 (18)	N12—H1N	0.8800
Ni1—N2	2.0526 (18)	N12—H2N	0.8801
Ni1—N21	2.1157 (16)	N21—C21	1.337 (3)
Ni1—N31	2.1250 (17)	N21—C25	1.344 (3)
Ni1—N41	2.1262 (17)	C21—C22	1.384 (3)
Ni1—N11	2.1316 (17)	C21—H21	0.9500
N1—C1	1.157 (3)	C22—C23	1.391 (3)
C1—S1	1.631 (2)	C22—H22	0.9500
N2—C2	1.159 (3)	C23—C24	1.387 (3)
C2—S2	1.636 (2)	C23—C26	1.490 (3)
O1—C3	1.405 (3)	C24—C25	1.378 (3)
O1—H1	0.8400	C24—H24	0.9500
C3—H3A	0.9800	C25—H25	0.9500
C3—H3B	0.9800	C26—N22	1.322 (3)
C3—H3C	0.9800	C26—S21	1.661 (2)
O2—C4	1.398 (4)	N22—H4N	0.8800
O2—H2	0.8400	N22—H3N	0.8801
C4—H4A	0.9800	N31—C35	1.339 (3)
C4—H4B	0.9800	N31—C31	1.342 (3)
C4—H4C	0.9800	C31—C32	1.377 (3)

O3—C5	1.388 (4)	C31—H31	0.9500
O3—H3	0.8400	C32—C33	1.385 (3)
C5—H5A	0.9800	C32—H32	0.9500
C5—H5B	0.9800	C33—C34	1.394 (3)
C5—H5C	0.9800	C33—C36	1.489 (3)
O4—C6	1.395 (5)	C34—C35	1.377 (3)
O4—H4	0.8400	C34—H34	0.9500
C6—H6A	0.9800	C35—H35	0.9500
C6—H6B	0.9800	C36—N32	1.315 (3)
C6—H6C	0.9800	C36—S31	1.657 (2)
O5—C7	1.341 (6)	N32—H5N	0.8801
O5—H5	0.8401	N32—H6N	0.8799
C7—H7A	0.9800	N41—C41	1.334 (3)
C7—H7B	0.9800	N41—C45	1.340 (3)
C7—H7C	0.9800	C41—C42	1.383 (3)
N11—C11	1.329 (3)	C41—H41	0.9500
N11—C15	1.344 (3)	C42—C43	1.385 (3)
C11—C12	1.379 (3)	C42—H42	0.9500
C11—H11	0.9500	C43—C44	1.389 (3)
C12—C13	1.385 (3)	C43—C46	1.501 (3)
C12—H12	0.9500	C44—C45	1.377 (3)
C13—C14	1.385 (3)	C44—H44	0.9500
C13—C16	1.496 (3)	C45—H45	0.9500
C14—C15	1.380 (3)	C46—N42	1.313 (3)
C14—H14	0.9500	C46—S41	1.656 (3)
C15—H15	0.9500	N42—H7N	0.8799
C16—N12	1.319 (3)	N42—H8N	0.8800
C16—S11	1.663 (3)		

N1—Ni1—N2	178.69 (7)	C16—N12—H1N	121.7
N1—Ni1—N21	90.21 (7)	C16—N12—H2N	127.8
N2—Ni1—N21	90.67 (7)	H1N—N12—H2N	110.4
N1—Ni1—N31	89.06 (7)	C21—N21—C25	117.90 (17)
N2—Ni1—N31	89.98 (7)	C21—N21—Ni1	121.02 (13)
N21—Ni1—N31	89.16 (6)	C25—N21—Ni1	121.08 (13)
N1—Ni1—N41	89.46 (7)	N21—C21—C22	122.89 (19)
N2—Ni1—N41	89.65 (7)	N21—C21—H21	118.6
N21—Ni1—N41	179.30 (7)	C22—C21—H21	118.6
N31—Ni1—N41	90.22 (7)	C21—C22—C23	118.92 (19)
N1—Ni1—N11	91.28 (7)	C21—C22—H22	120.5
N2—Ni1—N11	89.71 (7)	C23—C22—H22	120.5
N21—Ni1—N11	88.91 (6)	C24—C23—C22	118.20 (19)
N31—Ni1—N11	178.04 (6)	C24—C23—C26	120.74 (19)
N41—Ni1—N11	91.72 (7)	C22—C23—C26	121.04 (19)
C1—N1—Ni1	170.85 (17)	C25—C24—C23	119.27 (19)
N1—C1—S1	179.7 (2)	C25—C24—H24	120.4
C2—N2—Ni1	173.81 (17)	C23—C24—H24	120.4
N2—C2—S2	179.4 (2)	N21—C25—C24	122.78 (19)

C3—O1—H1	109.5	N21—C25—H25	118.6
O1—C3—H3A	109.5	C24—C25—H25	118.6
O1—C3—H3B	109.5	N22—C26—C23	115.3 (2)
H3A—C3—H3B	109.5	N22—C26—S21	124.16 (17)
O1—C3—H3C	109.5	C23—C26—S21	120.56 (17)
H3A—C3—H3C	109.5	C26—N22—H4N	122.5
H3B—C3—H3C	109.5	C26—N22—H3N	123.7
C4—O2—H2	109.5	H4N—N22—H3N	113.5
O2—C4—H4A	109.5	C35—N31—C31	117.33 (18)
O2—C4—H4B	109.5	C35—N31—Ni1	120.65 (14)
H4A—C4—H4B	109.5	C31—N31—Ni1	121.92 (14)
O2—C4—H4C	109.5	N31—C31—C32	123.0 (2)
H4A—C4—H4C	109.5	N31—C31—H31	118.5
H4B—C4—H4C	109.5	C32—C31—H31	118.5
C5—O3—H3	109.5	C31—C32—C33	119.5 (2)
O3—C5—H5A	109.5	C31—C32—H32	120.2
O3—C5—H5B	109.5	C33—C32—H32	120.2
H5A—C5—H5B	109.5	C32—C33—C34	117.7 (2)
O3—C5—H5C	109.5	C32—C33—C36	122.0 (2)
H5A—C5—H5C	109.5	C34—C33—C36	120.3 (2)
H5B—C5—H5C	109.5	C35—C34—C33	119.0 (2)
C6—O4—H4	109.5	C35—C34—H34	120.5
O4—C6—H6A	109.5	C33—C34—H34	120.5
O4—C6—H6B	109.5	N31—C35—C34	123.4 (2)
H6A—C6—H6B	109.5	N31—C35—H35	118.3
O4—C6—H6C	109.5	C34—C35—H35	118.3
H6A—C6—H6C	109.5	N32—C36—C33	116.1 (2)
H6B—C6—H6C	109.5	N32—C36—S31	124.75 (19)
C7—O5—H5	107.6	C33—C36—S31	119.16 (17)
O5—C7—H7A	107.6	C36—N32—H5N	118.1
O5—C7—H7B	110.9	C36—N32—H6N	122.8
H7A—C7—H7B	108.2	H5N—N32—H6N	119.1
O5—C7—H7C	112.6	C41—N41—C45	117.46 (18)
H7A—C7—H7C	108.2	C41—N41—Ni1	122.39 (14)
H7B—C7—H7C	109.3	C45—N41—Ni1	120.14 (14)
C11—N11—C15	116.96 (18)	N41—C41—C42	123.2 (2)
C11—N11—Ni1	119.87 (14)	N41—C41—H41	118.4
C15—N11—Ni1	123.18 (14)	C42—C41—H41	118.4
N11—C11—C12	123.6 (2)	C41—C42—C43	119.0 (2)
N11—C11—H11	118.2	C41—C42—H42	120.5
C12—C11—H11	118.2	C43—C42—H42	120.5
C11—C12—C13	119.3 (2)	C42—C43—C44	118.0 (2)
C11—C12—H12	120.3	C42—C43—C46	121.1 (2)
C13—C12—H12	120.3	C44—C43—C46	120.8 (2)
C14—C13—C12	117.7 (2)	C45—C44—C43	119.1 (2)
C14—C13—C16	121.8 (2)	C45—C44—H44	120.4
C12—C13—C16	120.5 (2)	C43—C44—H44	120.4
C15—C14—C13	119.2 (2)	N41—C45—C44	123.1 (2)

C15—C14—H14	120.4	N41—C45—H45	118.4
C13—C14—H14	120.4	C44—C45—H45	118.4
N11—C15—C14	123.3 (2)	N42—C46—C43	116.3 (2)
N11—C15—H15	118.4	N42—C46—S41	124.76 (18)
C14—C15—H15	118.4	C43—C46—S41	118.88 (18)
N12—C16—C13	114.9 (2)	C46—N42—H7N	125.7
N12—C16—S11	124.92 (18)	C46—N42—H8N	117.1
C13—C16—S11	120.23 (18)	H7N—N42—H8N	117.1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···S2^{i}	0.84	2.88	3.409 (2)	123
O1—H1···S11^{ii}	0.84	2.92	3.578 (2)	137
O2—H2···S31^{iii}	0.84	2.62	3.413 (3)	157
O3—H3···S1^{iv}	0.84	2.77	3.427 (2)	136
O3—H3···S31^{v}	0.84	2.93	3.576 (2)	135
C5—H5*A*···S31^{v}	0.98	3.03	3.632 (4)	121
O4—H4···O5	0.84	1.92	2.708 (5)	156
C6—H6*B*···S31^{vi}	0.98	2.73	3.566 (4)	143
O5—H5···S41^{vii}	0.84	2.51	3.216 (3)	142
C7—H7*A*···S41^{vii}	0.98	2.93	3.528 (5)	121
C11—H11···N1	0.95	2.52	3.063 (3)	117
C11—H11···S1^{viii}	0.95	2.73	3.442 (2)	133
C12—H12···S1^{viii}	0.95	2.96	3.542 (2)	121
C15—H15···N2	0.95	2.61	3.097 (3)	113
N12—H1*N*···O2	0.88	2.02	2.898 (3)	177
N12—H2*N*···S2^{ix}	0.88	2.58	3.446 (2)	171
C21—H21···N1	0.95	2.65	3.109 (3)	110
C25—H25···N2	0.95	2.66	3.122 (3)	111
C25—H25···S2^{x}	0.95	2.94	3.846 (2)	159
N22—H4*N*···S2^{xi}	0.88	2.64	3.4939 (19)	163
N22—H3*N*···O1	0.88	2.10	2.978 (3)	174
N32—H5*N*···O5	0.88	1.95	2.833 (3)	180
N32—H6*N*···S1^{vi}	0.88	2.64	3.478 (2)	159
C45—H45···S11^{ix}	0.95	2.89	3.673 (2)	141
N42—H7*N*···O3	0.88	2.08	2.957 (3)	173
N42—H8*N*···S1^{xii}	0.88	2.88	3.749 (2)	169

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