

Synthesis and crystal structure of *catena*-poly-[[bis(pyridine-4-carbonitrile- κN^1)cobalt(II)]-di- μ -thiocyanato- $\kappa^2 N:S;\kappa^2 S:N$]

Christian Näther*

Institut für Anorganische Chemie, Universität Kiel, Germany. *Correspondence e-mail: cnaether@ac.uni-kiel.de

Received 18 September 2026

Accepted 21 September 2026

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: synthesis; cobalt thiocyanate; pyridine-4-carbonitrile; chain compound; crystal structure.

CCDC reference: 2589650

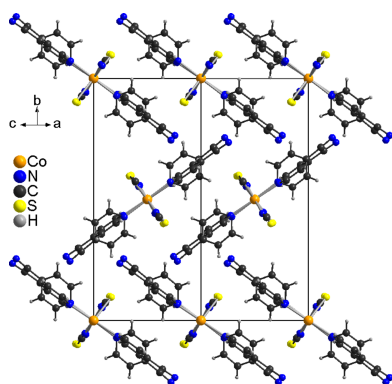
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The asymmetric unit of the title compound, $[\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2]_n$ ($\text{C}_6\text{H}_4\text{N}_2$ = pyridine-4-carbonitrile), consists of two crystallographically independent cobalt cations that are located on centers of inversion as well as two independent thiocyanate anions and two independent pyridine-4-carbonitrile coligands that occupy general positions. Each of the cobalt cations is sixfold coordinated by two N- and two S-bonding thiocyanate anions and two pyridine-4-carbonitrile coligands in a slightly distorted CoN_4S_2 octahedral geometry with an all-*trans* coordination. The cobalt cations are linked by pairs of μ -1,3-bridging anionic ligands into linear chains. Powder X-ray diffraction (PXRD) experiments indicate that the title compound was obtained as a pure phase. Moreover, comparison of the experimental X-ray powder pattern of the residue obtained after water removal from $[\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2]$ reported recently [Näther (2026). *Acta Cryst. E* **82**, 441–445] with the calculated powder pattern of the title compound proves that the latter crystalline phase has formed and indicates that a second modification with the same composition as that of the title compound might exist.

1. Chemical context

For many years, we and others have been interested in the synthesis, crystal structures and magnetic properties of transition-metal thiocyanate and selenocyanate coordination polymers in which the metal cations are linked by μ -1,3-bridging anionic ligands into one-dimensional or two-dimensional networks (Näther & Greve, 2003; Wöhlert *et al.*, 2013; Neumann *et al.*, 2018). In this context compounds based on Co^{II} are of special interest, because they can show one-dimensional or three-dimensional ferromagnetic ordering (Lescouëzec *et al.*, 2005; Mautner *et al.*, 2018; Wöhlert *et al.*, 2012; 2013; Rams *et al.*, 2020). In some cases such compounds are difficult to prepare and we therefore developed an alternative strategy in which precursor compounds with only terminally N-bonding thiocyanate anions and weakly bound coligands are heated. This frequently leads to the formation of compounds in which the metal cations are linked by bridging anionic ligands (Näther & Greve, 2003; Wriedt & Näther, 2010).

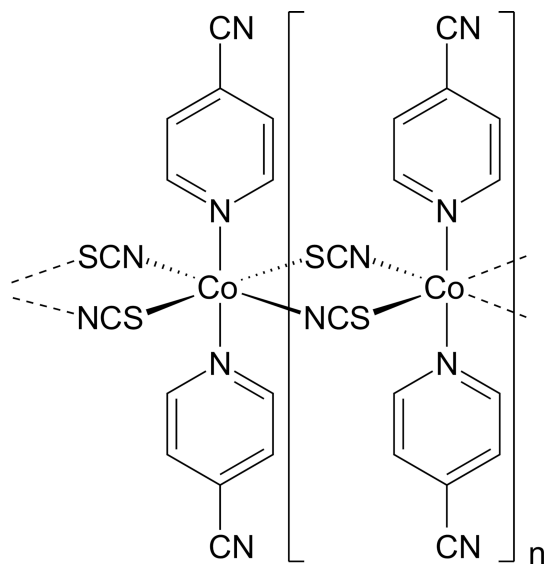
In this context, we have recently reported on a discrete aqua complex with the composition $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2$ ($\text{C}_6\text{H}_4\text{N}_2$ = pyridine-4-carbonitrile) in which the metal cations are octahedrally coordinated by two N-bonding thiocyanate anions, two pyridine-4-carbonitrile ligands and two water molecules. Thermogravimetric measurements reveal, that this complex decomposes in separate steps, in which compounds with the composition $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2$ and $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)$ are formed as intermediates. PXRD measurements



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of these residues reveal that crystalline phases have formed and that the residue obtained after the first mass loss consists of a mixture of two different crystalline phases, of which one might be isotypic to the corresponding Mn compound $\text{Mn}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2$ (Wellm *et al.*, 2020).



Starting from these results we tried to prepare single crystals of the two pyridine-4-carbonitrile-deficient coordination compounds, which led to the formation of crystals of the title compound, $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2$ (**I**), which were characterized by single crystal X-ray diffraction.

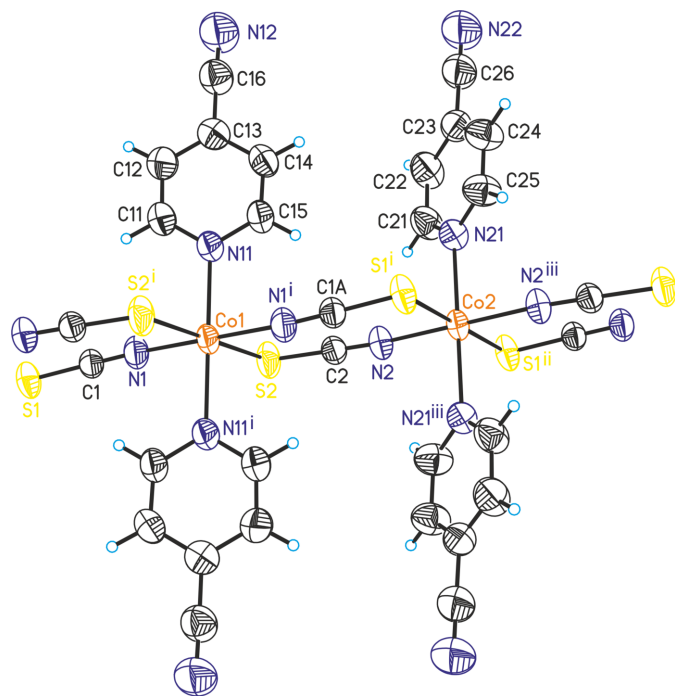


Figure 1
Crystal structure of (**I**) with labeling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) $x - 1, y, z - 1$; (ii) $-x + 2, -y + 1, -z + 1$; (iii) $-x + 1, -y + 1, -z$.

Table 1
Selected geometric parameters ($\text{\AA}$, $^\circ$).

Co1—N1	2.068 (2)	Co2—S1 ⁱ	2.6178 (6)
Co1—S2	2.5836 (7)	Co2—N2	2.0462 (19)
Co1—N11	2.181 (2)	Co2—N21	2.185 (2)
N1—Co1—S2	86.30 (6)	N2—Co2—S1 ⁱⁱ	92.99 (6)
N1 ⁱⁱ —Co1—S2	93.70 (6)	N2—Co2—S1 ⁱ	87.01 (6)
N1 ⁱⁱ —Co1—N11	89.37 (8)	N2—Co2—N21 ⁱⁱⁱ	89.60 (8)
N1—Co1—N11	90.63 (8)	N2—Co2—N21	90.40 (8)
N11 ⁱⁱⁱ —Co1—S2	92.18 (6)	N21—Co2—S1 ⁱ	88.87 (6)
N11—Co1—S2	87.81 (6)	N21—Co2—S1 ⁱⁱ	91.13 (6)

Symmetry codes: (i) $x - 1, y, z - 1$; (ii) $-x + 2, -y + 1, -z + 1$; (iii) $-x + 1, -y + 1, -z$.

2. Structural commentary

The asymmetric unit of (**I**) consists of two crystallographically independent cobalt cations that occupy centers of inversion as well as two crystallographically independent thiocyanate anions and two crystallographically independent pyridine-4-carbonitrile ligands that are located in general positions in space group $P2_1/c$. Each cobalt cation is sixfold coordinated by pairs of N- and S-bonding thiocyanate anions and two pyridine-4-carbonitrile ligands that coordinate with the pyridine atom to the metal centers in an all-*trans* CoN_4S_2 octahedral coordination environment (Fig. 1). Bond lengths and angles are comparable for both cobalt cations and deviate only slightly from the ideal values, which shows that the octahedra are slightly distorted (Table 1). The cobalt cations are linked by pairs of μ -1,3-bridging anionic ligands into linear chains that propagate along the $[101]$ direction (Fig. 2).

It is noted that the title compound is not isotypic to the corresponding Mn compound already reported in the literature, which crystallizes in the monoclinic space group $P2_1/n$ with $a = 5.7311$ (4) $\text{\AA}$, $b = 17.86665$ (15) $\text{\AA}$, $c = 8.5822$ (5) $\text{\AA}$ and $\beta = 107.624^\circ$ [$V = 837.5$ (3) $\text{\AA}^3$ at 195 K] (Wellm *et al.*, 2020). Surprisingly, a similar unit cell with the same space

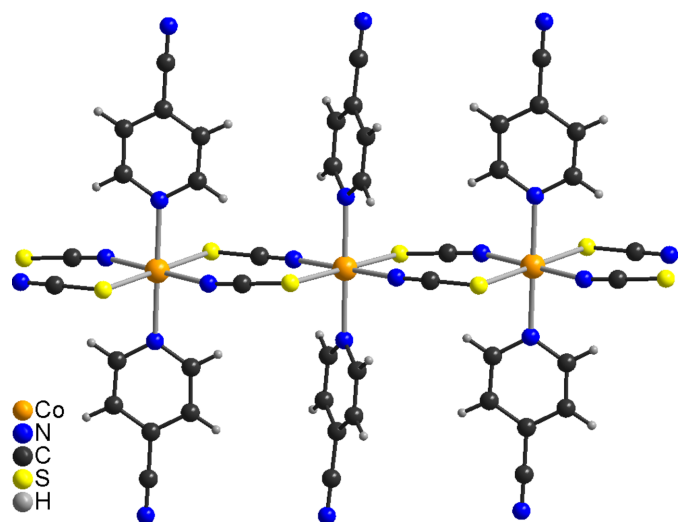


Figure 2
Fragment of the crystal structure of (**I**) with a view of part of a chain.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11 $\cdots$ N1	0.93	2.63	3.126 (4)	114
C15—H15 $\cdots$ N1 ⁱⁱ	0.93	2.59	3.106 (3)	115
C21—H21 $\cdots$ N2	0.93	2.61	3.134 (3)	116
C22—H22 $\cdots$ N12 ^{iv}	0.93	2.67	3.287 (4)	124
C24—H24 $\cdots$ S2 ^v	0.93	2.98	3.813 (3)	150
C25—H25 $\cdots$ N2 ⁱⁱⁱ	0.93	2.55	3.065 (4)	115

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

group can also be found for the title compound if some of the weak reflections are omitted. However, if the structure is refined in this smaller unit cell, the six-membered rings of the pyridine-4-carbonitrile are disordered over two orientations, which clearly shows that the larger unit cell is correct. In contrast, in the Mn compound with half of the unit-cell volume no disorder is observed, which shows that this unit cell is correct and that this modification is different from that of the title compound.

3. Supramolecular features

In the extended structure of (**I**), the [101] chains are packed in a way that is reminiscent of a sandwich-herringbone arrangement (Fig. 3). There are a number of C—H $\cdots$ N and C—H $\cdots$ S contacts (Table 2) but with long H $\cdots$ N and H $\cdots$ S distances and with angles far from linearity, indicating that these are very weak interactions.

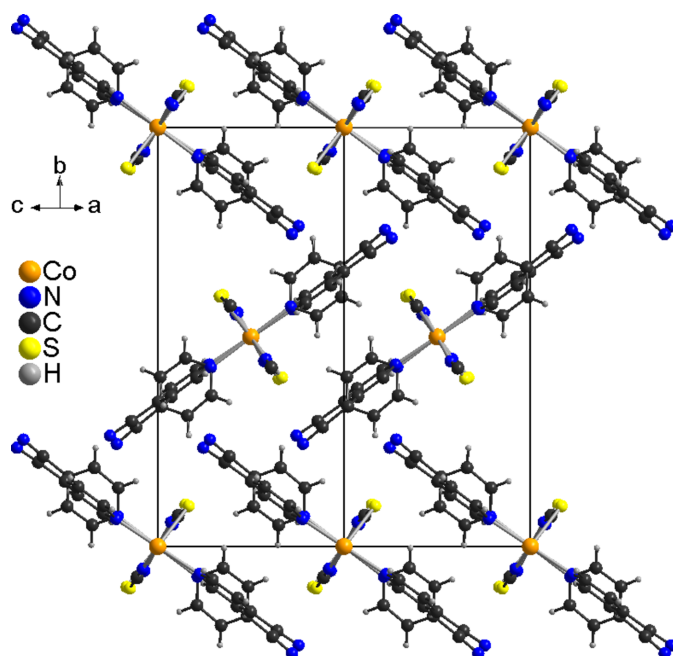


Figure 3

Crystal structure of (**I**) in a view along the [101] direction.

4. Database survey

It is noted that several coordination compounds with pyridine-4-carbonitrile and transition metal thiocyanates are already reported in the CSD [version 5.43, last update January 2026 (Groom *et al.*, 2016) searched using CONQUEST (Bruno *et al.*, 2002)]. Most of them are combined with Mn(NCS)₂. This includes discrete complexes with the composition Mn(NCS)₂(C₆H₄N₂)₄ (CSD refcode: OJEDOZ; Wellm *et al.*, 2020) and Mn(NCS)₂(C₆H₄N₂)₂(H₂O)₂ (OJEFAN and OJEFAN01; Wellm *et al.*, 2020), which crystallizes in two different modifications. Discrete aqua complexes with the composition Mn(NCS)₂(C₆H₄N₂)₂(H₂O)₂ and additional pyridine-4-carbonitrile as solvate molecules are also known (OJEFER and OJEFUH; Wellm *et al.*, 2020). Compounds with bridging anionic ligands with the composition Mn(NCS)₂(C₆H₄N₂)₂ (OJEFIV; Wellm *et al.*, 2020) and two isomers of Mn(NCS)₂(C₆H₄N₂) (OJEDUF and OJEDUF01; Wellm *et al.*, 2020) are also known.

With nickel, two compounds built up of discrete complexes are reported, *viz.* Ni(NCS)₂(C₆H₄N₂)₄ (UBUBOL; Clegg & Harrington, 2016) and Ni(NCS)₂(C₆H₄N₂)₂(H₂O)₂ (Näther, 2026). Fe(NCS)₂(C₆H₄N₂)₂(H₂O)₂(C₆H₄N₂)₂ (KAPQEA; Jochim *et al.*, 2017) also consists of discrete complexes with additional pyridine-4-carbonitrile molecules located in cavities of this structure.

Moreover, compounds with the composition Cd(NCS)₂(C₆H₄N₂)₂ (WUCLUB; Chen *et al.*, 2002) and Cu(NCS)₂(C₆H₄N₂)₂ (ABOVOF; Handy *et al.*, 2017) are known which exhibit the same ratio between metal thiocyanate and pyridine-4-carbonitrile as observed in the title compound. In both compounds the metal cations are linked by the anionic ligands into chains, but none of these compounds is isotypic to the title compound. The cadmium compound is isotypic to the corresponding manganese compound mentioned above (OJEFIV; Wellm *et al.*, 2020). Finally, in Cd(NCS)₂(C₆H₄N₂) (WUCMAI; Chen *et al.*, 2002) the pyridine-4-carbonitrile ligand acts as a bridging ligand. This compound is isotypic to one of the two modifications of Mn(NCS)₂(C₆H₄N₂) (OJEDUF01; Wellm *et al.*, 2020).

5. Synthesis and crystallization

Co(NCS)₂ and pyridine-4-carbonitrile were purchased from Sigma-Aldrich. 1.00 mmol (175.2 mg) Co(NCS)₂ and 2.00 mmol (208.2 mg) pyridine-4-carbonitrile were stirred in 1 ml of ethanol for 1 d. The precipitate was filtered off and dried in air. Single crystals of (**I**) in the form of light-red blocks were obtained using the same amount of reactants without stirring.

The asymmetric CN stretching vibration of the thiocyanate anions is observed at 2102 cm⁻¹ in the IR spectrum, in agreement with the bridging coordination of the anionic ligands (Fig. 4). Powder X-ray diffraction (PXRD) experiments show that the title compound was obtained as a pure phase (Fig. 5). Moreover, comparison of the experimental X-ray powder pattern of the residue obtained after water

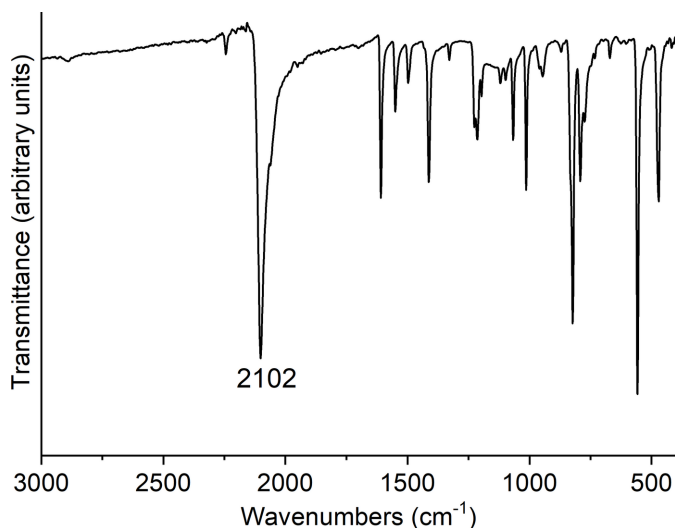


Figure 4
IR spectrum of (**I**) with the CN stretching vibration of the thiocyanate anion shown.

removal from $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2$ reported recently (Näther, 2026) with the calculated powder pattern of the title compound indicate that the title compound has formed in a mixture with a second and unknown modification of $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2$ (Fig. 6).

Powder X-ray diffraction measurements were performed using a Stoe STADI P transmission powder diffractometer with $\text{Cu } K\alpha_1$ radiation ($\lambda = 1.540598 \text{ \AA}$), a Johann-type $\text{Ge}(111)$ monochromator and a MYTHEN 1K detector from Dectris.

IR spectroscopy was done using an ATI Mattson Genesis Series FTIR Spectrometer, control software: *WINFIRST*, from ATI Mattson in ATR mode.

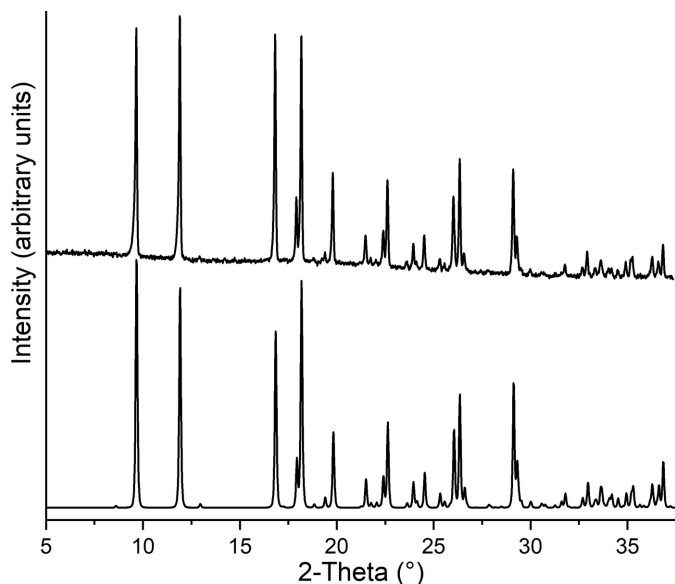


Figure 5
Experimental (top) and calculated (bottom) PXRD patterns for (**I**).

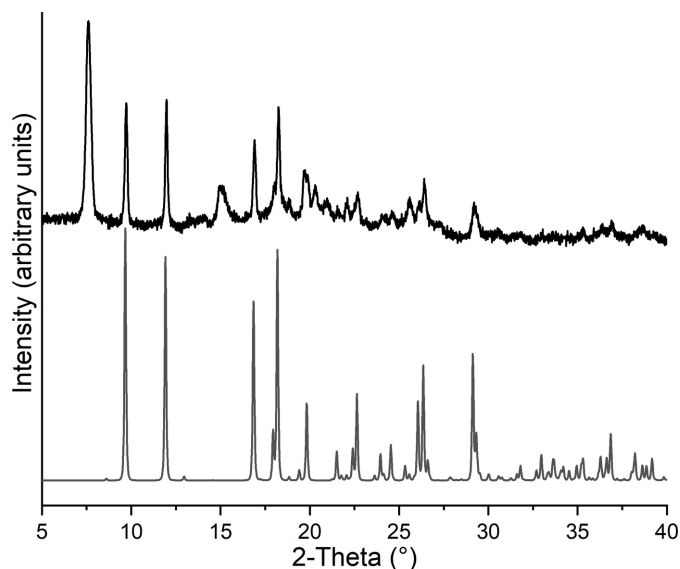


Figure 6
Experimental (top) PXRD pattern of $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2$ obtained by water removal from $\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2$ (Wellm *et al.*, 2020) and calculated (bottom) powder pattern for (**I**).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound hydrogen atoms were positioned with idealized geometry and were refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ using a riding model.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[\text{Co}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2]$
M_r	383.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	300
a, b, c (Å)	11.1023 (4), 18.2814 (8), 8.9315 (5)
β (°)	112.436 (3)
V (Å ³)	1675.57 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.28
Crystal size (mm)	$0.17 \times 0.12 \times 0.09$
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Numerical (<i>X-RED</i> and <i>X-SHAPE</i> ; Stoe, 2008)
$T_{\text{min}}, T_{\text{max}}$	0.710, 0.845
No. of measured, independent and observed [$I > 4\sigma(I)$] reflections	16251, 3288, 2401
R_{int}	0.043
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.036, 0.088, 1.07
No. of reflections	3288
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.38, -0.25

Computer programs: *X-Area* and *X-RED32* (Stoe, 2008), *SHELXT* (Sheldrick, 2015a), *SHELXL2016/6* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *SHELXTL* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 1999) and *pubCIF* (Westrip, 2010).

Acknowledgements

This work was supported by the State of Schleswig-Holstein.

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supporting information

Acta Cryst. (2026). E82, 1205-1209 [https://doi.org/10.1107/S2056989026009825]

Synthesis and crystal structure of *catena*-poly[[bis(pyridine-4-carbonitrile- κN^1)cobalt(II)]-di- μ -thiocyanato- $\kappa^2 N:S;\kappa^2 S:N$]

Christian Näther

Computing details

catena-Poly[[bis(pyridine-4-carbonitrile- κN^1)cobalt(II)]-di- μ -thiocyanato- $\kappa^2 N:S;\kappa^2 S:N$]

Crystal data

[Co(NCS)₂(C₆H₄N₂)₂]

$M_r = 383.31$

Monoclinic, $P2_1/c$

$a = 11.1023$ (4) Å

$b = 18.2814$ (8) Å

$c = 8.9315$ (5) Å

$\beta = 112.436$ (3)°

$V = 1675.57$ (14) Å³

$Z = 4$

$F(000) = 772$

$D_x = 1.520$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 13003 reflections

$\theta = 2.0$ – 28.4 °

$\mu = 1.28$ mm⁻¹

$T = 300$ K

Block, light red

$0.17 \times 0.12 \times 0.09$ mm

Data collection

Stoe IPDS 2

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus

Plane graphite monochromator

Detector resolution: 6.67 pixels mm⁻¹

ω scans

Absorption correction: numerical (X-Red and X-Shape; Stoe, 2008)

$T_{\min} = 0.710$, $T_{\max} = 0.845$

16251 measured reflections

3288 independent reflections

2401 reflections with $I > 4\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 2.0$ °

$h = -13 \rightarrow 13$

$k = -21 \rightarrow 22$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.088$

$S = 1.07$

3288 reflections

211 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.2371P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.38$ e Å⁻³

$\Delta\rho_{\min} = -0.25$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.000000	0.500000	0.500000	0.04672 (14)
Co2	0.500000	0.500000	0.000000	0.04134 (13)
N1	1.17221 (19)	0.44202 (12)	0.6006 (2)	0.0515 (5)
C1	1.2795 (2)	0.42552 (13)	0.6692 (3)	0.0416 (5)
S1	1.43258 (5)	0.40342 (4)	0.76597 (8)	0.05299 (18)
N2	0.67531 (18)	0.44698 (11)	0.0948 (2)	0.0480 (5)
C2	0.7798 (2)	0.42780 (13)	0.1701 (3)	0.0429 (5)
S2	0.92796 (6)	0.40021 (4)	0.27846 (8)	0.0588 (2)
N11	0.91226 (18)	0.43418 (12)	0.6354 (2)	0.0515 (5)
C11	0.9848 (3)	0.40288 (19)	0.7757 (4)	0.0703 (8)
H11	1.074005	0.411988	0.818576	0.084*
C12	0.9339 (3)	0.35758 (19)	0.8603 (4)	0.0702 (8)
H12	0.987944	0.336118	0.957045	0.084*
C13	0.8022 (3)	0.34469 (14)	0.7996 (3)	0.0543 (6)
C14	0.7265 (2)	0.37688 (15)	0.6556 (3)	0.0563 (6)
H14	0.636912	0.369148	0.611322	0.068*
C15	0.7847 (2)	0.42066 (16)	0.5777 (3)	0.0548 (6)
H15	0.732429	0.441945	0.479851	0.066*
C16	0.7433 (3)	0.29886 (17)	0.8840 (4)	0.0660 (7)
N12	0.6942 (3)	0.26440 (17)	0.9497 (4)	0.0947 (9)
N21	0.42045 (19)	0.42792 (10)	0.1347 (3)	0.0486 (5)
C21	0.4642 (3)	0.35993 (15)	0.1750 (4)	0.0633 (7)
H21	0.534751	0.344242	0.151511	0.076*
C22	0.4097 (3)	0.31194 (17)	0.2500 (4)	0.0708 (8)
H22	0.443326	0.264979	0.276604	0.085*
C23	0.3053 (3)	0.33407 (15)	0.2850 (3)	0.0593 (7)
C24	0.2607 (3)	0.40443 (17)	0.2465 (4)	0.0672 (8)
H24	0.191268	0.421650	0.270553	0.081*
C25	0.3206 (3)	0.44875 (15)	0.1719 (4)	0.0624 (7)
H25	0.289582	0.496223	0.145920	0.075*
C26	0.2421 (3)	0.28496 (19)	0.3578 (4)	0.0767 (9)
N22	0.1929 (3)	0.2449 (2)	0.4133 (4)	0.1074 (11)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0261 (2)	0.0694 (3)	0.0399 (3)	0.0037 (2)	0.00720 (19)	−0.0001 (2)
Co2	0.0275 (2)	0.0449 (2)	0.0449 (3)	0.00325 (17)	0.00625 (18)	0.0008 (2)
N1	0.0356 (11)	0.0663 (13)	0.0450 (12)	0.0026 (10)	0.0068 (9)	−0.0043 (10)

C1	0.0342 (12)	0.0482 (13)	0.0390 (12)	0.0004 (9)	0.0102 (10)	−0.0044 (10)
S1	0.0308 (3)	0.0583 (4)	0.0597 (4)	0.0074 (3)	0.0059 (3)	−0.0112 (3)
N2	0.0322 (10)	0.0524 (11)	0.0503 (12)	0.0033 (9)	0.0058 (9)	−0.0041 (10)
C2	0.0347 (12)	0.0513 (13)	0.0409 (13)	−0.0002 (10)	0.0123 (10)	−0.0039 (11)
S2	0.0333 (3)	0.0803 (5)	0.0525 (4)	0.0156 (3)	0.0050 (3)	−0.0081 (3)
N11	0.0355 (10)	0.0697 (14)	0.0470 (12)	0.0025 (9)	0.0132 (9)	−0.0003 (10)
C11	0.0405 (14)	0.103 (2)	0.0613 (17)	0.0044 (15)	0.0129 (12)	0.0164 (17)
C12	0.0526 (16)	0.092 (2)	0.0625 (18)	0.0084 (15)	0.0186 (14)	0.0204 (16)
C13	0.0560 (16)	0.0497 (14)	0.0602 (16)	−0.0005 (12)	0.0255 (13)	−0.0054 (12)
C14	0.0417 (13)	0.0624 (15)	0.0628 (17)	−0.0056 (12)	0.0177 (12)	−0.0051 (14)
C15	0.0381 (12)	0.0686 (16)	0.0517 (15)	0.0015 (12)	0.0105 (11)	0.0002 (13)
C16	0.0625 (17)	0.0579 (16)	0.075 (2)	−0.0046 (14)	0.0229 (15)	0.0040 (15)
N12	0.085 (2)	0.087 (2)	0.106 (2)	−0.0131 (17)	0.0302 (18)	0.0300 (19)
N21	0.0444 (11)	0.0464 (11)	0.0539 (12)	−0.0002 (9)	0.0174 (10)	−0.0003 (9)
C21	0.0505 (15)	0.0551 (15)	0.086 (2)	0.0088 (12)	0.0282 (14)	0.0146 (15)
C22	0.0577 (16)	0.0540 (16)	0.097 (2)	0.0047 (13)	0.0255 (16)	0.0192 (16)
C23	0.0545 (16)	0.0630 (16)	0.0567 (17)	−0.0097 (13)	0.0171 (13)	0.0045 (14)
C24	0.0701 (19)	0.0651 (17)	0.080 (2)	0.0045 (15)	0.0438 (17)	0.0037 (15)
C25	0.0720 (18)	0.0513 (14)	0.0772 (19)	0.0079 (13)	0.0433 (16)	0.0034 (14)
C26	0.0657 (19)	0.081 (2)	0.081 (2)	−0.0086 (16)	0.0247 (17)	0.0157 (18)
N22	0.087 (2)	0.118 (3)	0.117 (3)	−0.019 (2)	0.038 (2)	0.039 (2)

Geometric parameters (Å, °)

Co1—N1 ⁱ	2.068 (2)	C12—H12	0.9300
Co1—N1	2.068 (2)	C12—C13	1.371 (4)
Co1—S2	2.5836 (7)	C13—C14	1.372 (4)
Co1—S2 ⁱ	2.5836 (7)	C13—C16	1.440 (4)
Co1—N11 ⁱ	2.181 (2)	C14—H14	0.9300
Co1—N11	2.181 (2)	C14—C15	1.373 (4)
Co2—S1 ⁱⁱ	2.6178 (6)	C15—H15	0.9300
Co2—S1 ⁱ	2.6178 (6)	C16—N12	1.132 (4)
Co2—N2 ⁱⁱⁱ	2.0462 (19)	N21—C21	1.333 (3)
Co2—N2	2.0462 (19)	N21—C25	1.329 (3)
Co2—N21	2.185 (2)	C21—H21	0.9300
Co2—N21 ⁱⁱⁱ	2.185 (2)	C21—C22	1.376 (4)
N1—C1	1.153 (3)	C22—H22	0.9300
C1—S1	1.636 (2)	C22—C23	1.372 (4)
N2—C2	1.151 (3)	C23—C24	1.374 (4)
C2—S2	1.638 (2)	C23—C26	1.438 (4)
N11—C11	1.333 (3)	C24—H24	0.9300
N11—C15	1.333 (3)	C24—C25	1.372 (4)
C11—H11	0.9300	C25—H25	0.9300
C11—C12	1.380 (4)	C26—N22	1.135 (4)
N1 ⁱ —Co1—N1	180.0	C15—N11—Co1	121.45 (17)
N1—Co1—S2	86.30 (6)	C15—N11—C11	117.1 (2)
N1 ⁱ —Co1—S2 ⁱ	86.29 (6)	N11—C11—H11	118.5

N1 ⁱ —Co1—S2	93.70 (6)	N11—C11—C12	123.1 (3)
N1—Co1—S2 ⁱ	93.71 (6)	C12—C11—H11	118.5
N1 ⁱ —Co1—N11 ⁱ	90.63 (8)	C11—C12—H12	120.5
N1 ⁱ —Co1—N11	89.37 (8)	C13—C12—C11	119.0 (3)
N1—Co1—N11	90.63 (8)	C13—C12—H12	120.5
N1—Co1—N11 ⁱ	89.37 (8)	C12—C13—C14	118.5 (3)
S2—Co1—S2 ⁱ	180.00 (2)	C12—C13—C16	121.4 (3)
N11 ⁱ —Co1—S2 ⁱ	87.82 (6)	C14—C13—C16	120.1 (3)
N11 ⁱ —Co1—S2	92.18 (6)	C13—C14—H14	120.5
N11—Co1—S2 ⁱ	92.18 (6)	C13—C14—C15	119.1 (2)
N11—Co1—S2	87.81 (6)	C15—C14—H14	120.5
N11 ⁱ —Co1—N11	180.0	N11—C15—C14	123.3 (2)
S1 ⁱⁱ —Co2—S1 ⁱ	180.00 (3)	N11—C15—H15	118.4
N2—Co2—S1 ⁱ	92.99 (6)	C14—C15—H15	118.4
N2—Co2—S1 ⁱⁱ	87.01 (6)	N12—C16—C13	177.9 (4)
N2 ⁱⁱⁱ —Co2—S1 ⁱⁱ	92.99 (6)	C21—N21—Co2	121.93 (18)
N2 ⁱⁱⁱ —Co2—S1 ⁱ	87.01 (6)	C25—N21—Co2	121.07 (17)
N2 ⁱⁱⁱ —Co2—N2	180.00 (10)	C25—N21—C21	116.9 (2)
N2—Co2—N21 ⁱⁱⁱ	89.60 (8)	N21—C21—H21	118.5
N2—Co2—N21	90.40 (8)	N21—C21—C22	122.9 (3)
N2 ⁱⁱⁱ —Co2—N21 ⁱⁱⁱ	90.40 (8)	C22—C21—H21	118.5
N2 ⁱⁱⁱ —Co2—N21	89.60 (8)	C21—C22—H22	120.3
N21 ⁱⁱⁱ —Co2—S1 ⁱ	88.87 (6)	C23—C22—C21	119.3 (3)
N21 ⁱⁱⁱ —Co2—S1 ⁱⁱ	91.13 (6)	C23—C22—H22	120.3
N21—Co2—S1 ⁱⁱ	88.87 (6)	C22—C23—C24	118.3 (3)
N21—Co2—S1 ⁱ	91.13 (6)	C22—C23—C26	121.3 (3)
N21 ⁱⁱⁱ —Co2—N21	180.0	C24—C23—C26	120.4 (3)
C1—N1—Co1	164.1 (2)	C23—C24—H24	120.7
N1—C1—S1	179.0 (2)	C25—C24—C23	118.6 (3)
C1—S1—Co2 ^{iv}	100.25 (8)	C25—C24—H24	120.7
C2—N2—Co2	166.71 (19)	N21—C25—C24	123.9 (3)
N2—C2—S2	179.5 (2)	N21—C25—H25	118.0
C2—S2—Co1	100.52 (9)	C24—C25—H25	118.0
C11—N11—Co1	121.36 (17)	N22—C26—C23	178.4 (4)
Co1—N11—C11—C12	−176.3 (2)	C15—N11—C11—C12	0.6 (5)
Co1—N11—C15—C14	177.0 (2)	C16—C13—C14—C15	179.6 (3)
Co2—N21—C21—C22	−175.4 (2)	N21—C21—C22—C23	0.3 (5)
Co2—N21—C25—C24	175.5 (2)	C21—N21—C25—C24	−0.8 (5)
N11—C11—C12—C13	−1.0 (5)	C21—C22—C23—C24	−1.4 (5)
C11—N11—C15—C14	0.1 (4)	C21—C22—C23—C26	177.7 (3)
C11—C12—C13—C14	0.7 (5)	C22—C23—C24—C25	1.4 (4)
C11—C12—C13—C16	−179.0 (3)	C23—C24—C25—N21	−0.3 (5)
C12—C13—C14—C15	0.0 (4)	C25—N21—C21—C22	0.8 (4)
C13—C14—C15—N11	−0.4 (4)	C26—C23—C24—C25	−177.7 (3)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C11—H11 $\cdots$ N1	0.93	2.63	3.126 (4)	114
C15—H15 $\cdots$ N1 ⁱ	0.93	2.59	3.106 (3)	115
C21—H21 $\cdots$ N2	0.93	2.61	3.134 (3)	116
C22—H22 $\cdots$ N12 ^v	0.93	2.67	3.287 (4)	124
C24—H24 $\cdots$ S2 ^{vi}	0.93	2.98	3.813 (3)	150
C25—H25 $\cdots$ N2 ⁱⁱⁱ	0.93	2.55	3.065 (4)	115

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