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$Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ [abpt is 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole]: structural characterization of polymorphs A and B

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The synthesis and structures of bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)cobalt(II), $[Co(NCS)_2(C_{12}H_{10}N_6)_2]$ or $Co(NCS)_2(abpt)_2$, and bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)nickel(II), $[Ni(NCS)_2(C_{12}H_{10}N_6)_2]$ or $Ni(NCS)_2(abpt)_2$, are reported. In both cases, two polymorphs, **A** and **B**, were identified and structurally characterized. For both polymorphs, the structures obtained with the different metals, *i.e.* Co^{II} or Ni^{II}, were found to be isostructural. All of the structures contained an intramolecular N—H···N hydrogen bond, C—H···N interactions and π–π stacking interactions. No structural evidence was observed for a thermal spin crossover for either of the $Co(NCS)_2(abpt)_2$ polymorphs between 300 (2) and 120 (2) K.

1. Introduction

The bidentate ligand 4-amino-3,5-bis(pyridine-2-yl)-1,2,4-triazole (abpt) has been found to form mononuclear complexes, as well as single- or double-bridged dinuclear complexes, with a variety of metals (for examples, see Dupouy *et al.*, 2008; White *et al.*, 2009; Li *et al.*, 2011). Amongst these, a number of Fe^{II} complexes have been synthesized and studied because of their interesting polymorphism and spin-crossover behaviour. Perhaps the most studied is the $Fe(NCS)_2(abpt)_2$ complex, of which there are four known polymorphs, denoted **A**–**D**, all of which display different magnetic behaviour. Three of the polymorphs, *i.e.* **A** (Moliner *et al.*, 1999; Sheu *et al.*, 2009; Mason *et al.*, 2016), **C** (Sheu *et al.*, 2009; Shih *et al.*, 2010) and **D** (Sheu *et al.*, 2009, 2012; Mason *et al.*, 2021), undergo at least a partial thermal spin crossover under ambient pressure, while polymorph **B** (Gaspar *et al.*, 2003) only undergoes a thermal spin crossover at pressures above 4.4 kbar (1 bar = 10^5 Pa). All of the three polymorphs which display at least a partial thermal spin crossover also show light-induced excited-spin-state trapping (LIESST) at low temperature. While three of the polymorphs (**A**, **B** and **D**) are known to undergo a pressure-induced spin crossover at room temperature (Mason *et al.*, 2016, 2021), polymorph **C** has not been studied under pressure at room temperature. To date, $Co(NCS)_2(abpt)_2$ is the only other $M(NCS)_2(abpt)_2$ complex containing a transition metal for which any structures have been reported. Like the Fe analogue, this has also been found to display polymorphism, with two different polymorphs of $Co(NCS)_2(abpt)_2$ reported at room temperature. These will be referred to as $Co(NCS)_2(abpt)_2$ polymorphs **B** (Peng *et al.*, 2006) and **D** (Chen & Peng, 2007) throughout, as they are isostructural with

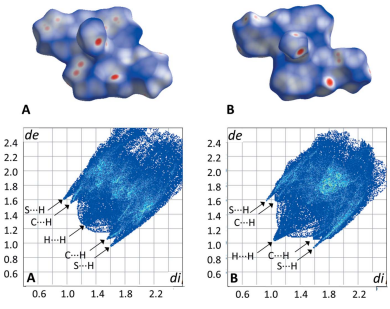


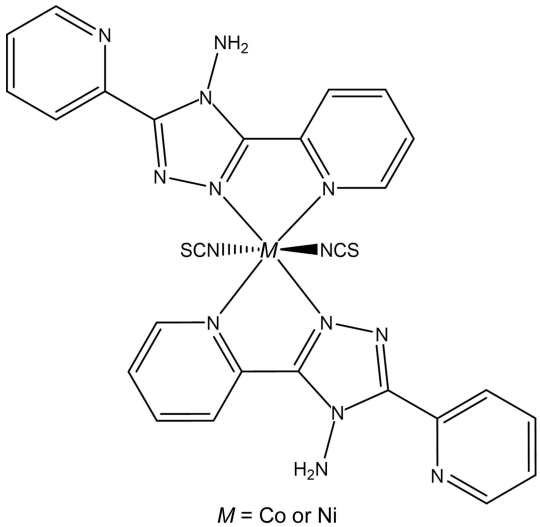
Table 1
Experimental details.

For all structures: monoclinic, $P2_1/n$, $Z = 2$. Experiments were carried out at 120 K with Mo $K\alpha$ radiation. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 1999–2013). Refinement was on 202 parameters. H atoms were treated by a mixture of independent and constrained refinement.

	$Co(NCS)_2(abpt)_2$, Polymorph **A**	$Co(NCS)_2(abpt)_2$, Polymorph **B**	$Ni(NCS)_2(abpt)_2$, Polymorph **A**	$Ni(NCS)_2(abpt)_2$, Polymorph **B**
Crystal data				
Chemical formula	$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$	$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$	$[Ni(NCS)_2(C_{12}H_{10}N_6)_2]$	$[Ni(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r	651.61	651.61	651.39	651.39
a, b, c (Å)	8.4792 (6), 10.1307 (7), 16.3774 (11)	11.4978 (5), 9.5235 (4), 12.7179 (5)	8.4041 (7), 10.0681 (9), 16.2360 (14)	11.5860 (14), 9.5489 (12), 12.8132 (16)
β (°)	93.485 (1)	100.771 (1)	93.060 (2)	100.806 (2)
V (Å^3)	1404.22 (17)	1368.07 (10)	1371.8 (2)	1392.4 (3)
μ (mm^{-1})	0.81	0.83	0.91	0.89
Crystal size (mm)	0.24 × 0.16 × 0.11	0.48 × 0.22 × 0.1	0.2 × 0.12 × 0.08	0.2 × 0.13 × 0.04
Data collection				
Diffractometer	Bruker SMART CCD 1K area detector	Bruker SMART CCD 1K area detector	Bruker D8 VENTURE	Bruker SMART CCD 1K area detector
T_{min}, T_{max}	0.793, 0.919	0.755, 0.884	0.781, 0.936	0.746, 0.948
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13341, 2884, 2383	13084, 2799, 2363	15450, 2819, 2161	12077, 2552, 1666
R_{int}	0.044	0.037	0.046	0.116
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625	0.625	0.602
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.093, 1.06	0.028, 0.065, 1.03	0.037, 0.085, 1.02	0.058, 0.136, 1.06
No. of reflections	2884	2799	2819	2552
No. of restraints	1	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.27	0.26, −0.39	0.48, −0.27	0.61, −0.66

Computer programs: *SMART*, *APEX2*, *SAINT* and *SAINT-Plus* (Bruker, 1999–2013), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

$Fe(NCS)_2(abpt)_2$ polymorphs **B** and **D**. The structures of two polymorphs, **A** and **B**, of both $Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ are reported herein (see Scheme 1).



M = Co or Ni
Scheme 1

2. Experimental

2.1. Synthesis

The synthesis of $M(NCS)_2(abpt)_2$, where *M* is Co or Ni, was carried out using a slow-diffusion method with methanol–water solutions as reported previously (Sheu *et al.*, 2009).

All chemicals were obtained from Sigma–Aldrich and used as supplied. $CoSO_4{\cdot}7H_2O$ (1 mmol, 0.281 g) or $NiSO_4{\cdot}6H_2O$ (1 mmol, 0.263 g) and KNCS (2 mmol, 0.194 g) were stirred in methanol (10 ml) for 15 min. A pale-yellow insoluble K_2SO_4 precipitate was removed by filtration and deionized water (10 ml) was added to the remaining clear solution. Abpt (2 mmol, 0.477 g) was dissolved in methanol (20 ml) and placed in a narrow (<5 cm) Schlenk tube. The M^{2+}/NCX^- solution was very carefully pipetted at the bottom of the Schlenk tube to form a lower more dense layer below the abpt solution. Immediately, a coloured band formed at the interface between the two layers containing the target complex. The Schlenk tube was left undisturbed and single crystals suitable for X-ray diffraction studies had formed within one week to one month later.

2.2. Refinement

Details of the crystallographic data collections are given in Table 1. All H atoms, apart from the N—H hydrogens, were positioned geometrically and refined using a riding model. The N—H hydrogens were located in a difference Fourier map (FDM) wherever feasible.

3. Results and discussion

The structure of $Co(NCS)_2(abpt)_2$ polymorph **B** has already been reported at room temperature and is consistent with that reported here (Peng *et al.*, 2006). The main structural features of all four structures are very similar: they all crystallized in the monoclinic space group $P2_1/n$ with half a molecule in the

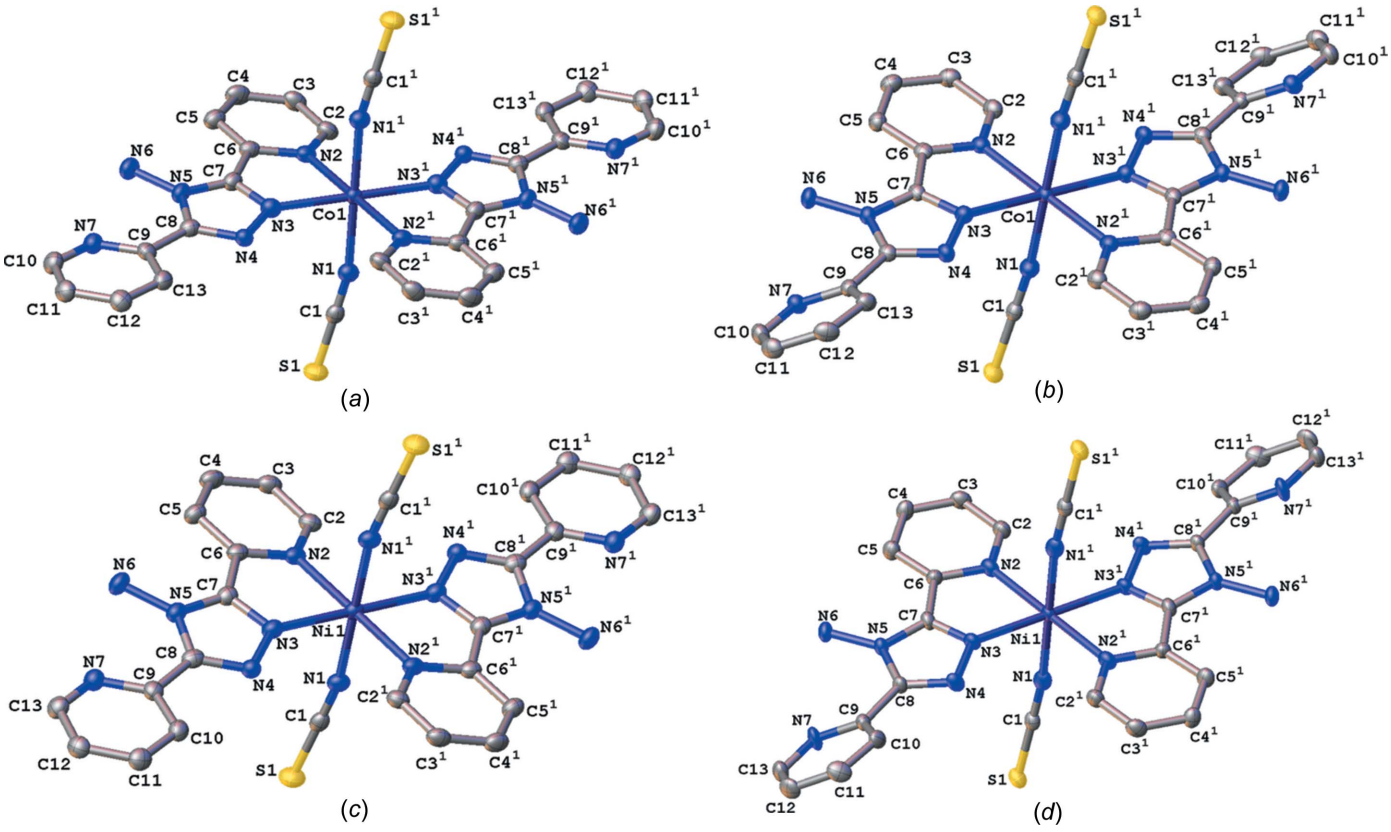


Figure 1
Illustration of the structures of $Co(NCS)_2(abpt)_2$ polymorphs (*a*) **A** and (*b*) **B**, and $Ni(NCS)_2(abpt)_2$ polymorphs (*c*) **A** and (*d*) **B**, with the atomic numbering schemes depicted. H atoms have been omitted for clarity. [Symmetry code: (i) $-x+1, -y+1, -z+1$.]

asymmetric unit ($Z' = 0.5$) (Fig. 1). Each of the four complexes consists of an approximately octahedrally coordinated metal centre (Co^{II} or Ni^{II}) coordinated to six N atoms, one from each of the NCS^- ligands and two from each abpt ligand (one pyridyl and one triazole N atom). Each of the structures contains an intramolecular N—H···N hydrogen bond between the NH_2 group on the triazole ring and the N atom of the uncoordinated pyridyl ring, as well as two intramolecular C—H···N interactions, one between a pyridyl C—H group and the N atom of the NH_2 group attached to the triazole ring, and a second between a pyridyl C—H group and the uncoordinated N atom on the triazole group (Table 2).

Table 2
Hydrogen-bond geometry (Å, °) for $Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ at 120 (2) K.

Structure	Polymorph	*D*—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
$Co(NCS)_2(abpt)_2$	**A**	N6—H6*B*···N7	0.90 (3)	2.14 (3)	2.861 (3)	136 (3)
		C5—H5···N6	0.95	2.53	3.135 (4)	122
		C2—H2···N4^{i}	0.95	2.67	3.467 (3)	142
	B	N6—H6*B*···N7	0.90 (2)	2.41 (2)	2.914 (2)	115.6 (16)
		C5—H5···N6	0.95	2.46	3.084 (2)	123
		C2—H2···N2^{i}	0.95	2.66	3.482 (2)	145
$Ni(NCS)_2(abpt)_2$	**A**	N6—H6*B*···N7	0.88 (3)	2.14 (3)	2.848 (3)	137 (3)
		C5—H5···N6	0.95	2.52	3.124 (4)	122
		C2—H2···N4^{ii}	0.95	2.55	3.347 (3)	141
	B	N6—H6*B*···N7	0.84 (6)	2.52 (5)	2.950 (6)	112 (4)
		C5—H5···N6	0.95	2.48	3.104 (7)	123
		C2—H2···N4^{ii}	0.95	2.59	3.403 (7)	144

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

The pair of **A** polymorphs of the Co^{II} or Ni^{II} structures are isostructural with each other, and are also isostructural with the previously reported $Fe(NCS)_2(abpt)_2$ polymorph **A** structure (Moliner *et al.*, 1999; Sheu *et al.*, 2009; Mason *et al.*, 2016). In addition to the previously mentioned N—H···N hydrogen bonding and C—H···N interactions, the structures contain intermolecular π–π stacking between pairs of molecules and involving the two pyridyl rings at each end of the abpt ligand interacting with the two pyridyl rings on an adjacent abpt ligand, creating a one-dimensional chain through the structure (Table 3 and Fig. 2).

As seen for the pair of polymorph **A** structures, the two polymorph **B** structures were also isostructural with each other and with the previously reported $Fe(NCS)_2(abpt)_2$ polymorph **B** structure (Gaspar *et al.*, 2003; Mason *et al.*, 2021). The structures of polymorph **B** also display π–π interactions, but in this case each of the pyridyl rings on the abpt ligand is involved in a π–π interaction to a pyridyl ring on a different abpt ligand, creating a three-dimensional network of interactions in the structure (Table 3 and Fig. 2). Along with the difference in the form of the π–π interactions between the polymorph **A** and polymorph **B** structures, the other main difference is the twist between the two rings on the abpt ligands. In the case of **A**, the twist between the rings is ∼9°, while for **B**,

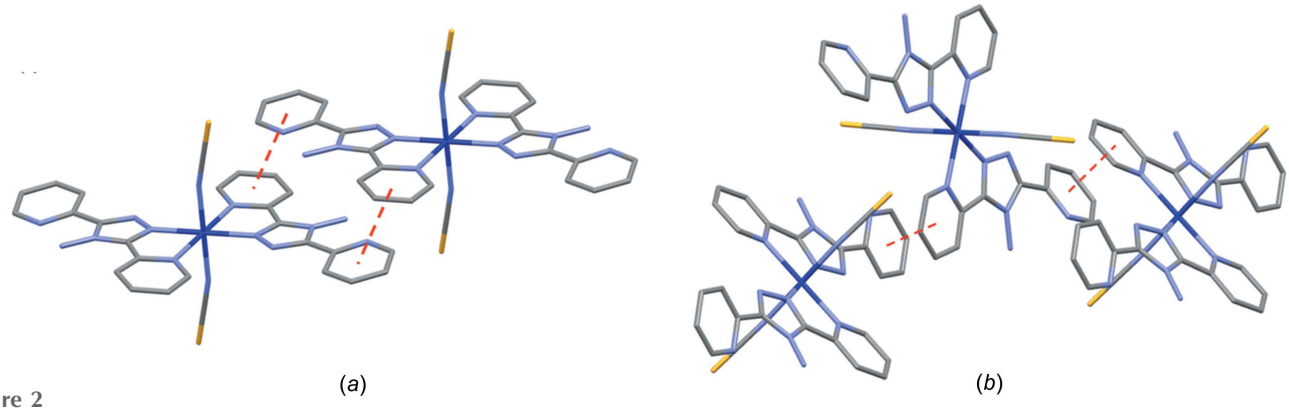


Figure 2
Illustration of the π–π stacking interactions as red dashed lines for one abpt ligand in (*a*) polymorph **A** (*b*) polymorph **B**.

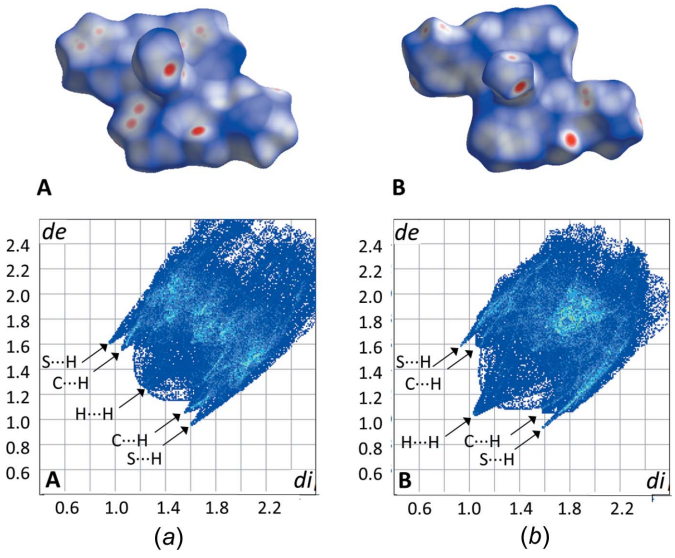


Figure 3
The Hirshfeld surface plot and fingerprint plot for (*a*) polymorph **A** and (*b*) polymorph **B** for $Co(NCS)_2(abpt)_2$. The Ni plots for the same respective polymorphs are essentially identical.

the twist between the rings is ∼35° (Table 4). This is likely to be the reason for the significantly different π–π stacking, as the larger twist in **B** would prevent both rings on one abpt ligand being correctly orientated to interact with both rings on a single abpt ligand on an adjacent molecule.

Table 3
π–π stacking interactions (Å) for $Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ at 120 (2) K.

Structure	Polymorph	Plane 1	Plane 2	Centroid-to-centroid distance	Shift distance
$Co(NCS)_2(abpt)_2$	**A**	N2,C2,C3,C4,C5,C6	N7,C9,C10,C11,C12,C13^{i}	3.63	1.31
		N7,C9,C10,C11,C12,C13	N2,C2,C3,C4,C5,C6^{i}	3.63	1.31
	B	N2,C2,C3,C4,C5,C6	N7,C9,C10,C11,C12,C13^{ii}	3.68	1.34
		N7,C9,C10,C11,C12,C13	N2,C2,C3,C4,C5,C6^{iii}	3.68	1.34
$Ni(NCS)_2(abpt)_2$	**A**	N2,C2,C3,C4,C5,C6	N7,C9,C10,C11,C12,C13^{i}	3.64	1.34
		N7,C9,C10,C11,C12,C13	N2,C2,C3,C4,C5,C6^{i}	3.64	1.34
	B	N2,C2,C3,C4,C5,C6	N7,C9,C10,C11,C12,C13^{ii}	3.72	1.41
		N7,C9,C10,C11,C12,C13	N2,C2,C3,C4,C5,C6^{iii}	3.72	1.41

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

Table 4
Twist and fold angles between planes calculated through the six atoms of the two rings on the abpt ligand at 120 (2) K.

Compound	Polymorph	Twist angle (°)	Fold angle (°)
$Co(NCS)_2(abpt)_2$	**A**	8.99 (8)	99.0 (8)
	B	35.25 (6)	142.50 (19)
$Ni(NCS)_2(abpt)_2$	**A**	9.39 (8)	96.7 (8)
	B	34.64 (17)	142.8 (6)

Table 5
Co—N distances for $Co(NCS)_2(abpt)_2$ at 120 (2) and 300 (2) K.

Polymorph	*T* (K)	Co1—N1	Co1—N2	Co1—N3
A	120	2.116 (2)	2.166 (2)	2.088 (2)
	300	2.113 (5)	2.164 (4)	2.093 (5)
B	120	2.0987 (15)	2.1616 (15)	2.1138 (14)
	300	2.102 (2)	2.166 (2)	2.1161 (18)

The Hirshfeld fingerprint plots (Turner *et al.*, 2017) for the two polymorphs highlight the differences between the two structures (Fig. 3). The plots are only shown for the Co polymorphs **A** and **B**, as the plots for the Ni polymorphs **A** and **B** were essentially identical to those of the respective Co polymorphs. The shapes of the two plots are clearly slightly different, although given that the structures are polymorphs, it is unsurprising that they show the same main short contacts. For both polymorphs, the S···H contacts are quite pronounced, with a similar shape and position. However, in the case of **A**, the C···H contacts are more pronounced than is seen for **B**, while the H···H contacts for **A** are less pronounced than observed for **B**. Examining the Hirshfeld surfaces for both compounds, the greater number of red spots on the surface of **A** than for **B** indicates that **A** has more short contacts.

Given that $Fe(NCS)_2(abpt)_2$ polymorph **A** was shown to have a spin transition upon cooling (Moliner *et al.*, 1999; Sheu *et al.*, 2009; Mason *et al.*, 2016), the data for Co^{II} d^7 polymorphs **A** and **B** were also measured at 300 (2) K (Table S1 in the supporting

information). Examining the Co—N bond lengths showed them to be essentially identical to the 120 (2) K structure and indicate that no spin transition had occurred over this temperature range (Table 5). In the case of Ni^{II}, the complex is d^8 so no spin transition would be possible.

4. Conclusions

The synthesis and structures of $Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ are reported. Two polymorphs were identified for each of the complexes, **A** and **B**, and the pairs of polymorphs with the different metal centres were found to be isostructural. All of the structures contained intramolecular N—H···N hydrogen bonding, intramolecular C—H···N interactions and π–π stacking. There are identifiable differences between the two polymorph structures. Firstly, the twist angle between the two six-membered rings on one abpt ligand was ∼9° for polymorph **A** and ∼35° for polymorph **B**. Secondly, the nature of the π–π stacking interactions was significantly different, presumably due to the differing twist angles of the rings. In the case of **A**, both rings on one abpt ligand form π–π stacking interactions with both rings on an abpt ligand on an adjacent molecule, while for **B**, each of the rings on the abpt ligand forms π–π stacking interactions with a ring on different abpt ligands in adjacent molecules. Variable-temperature studies on d^7 $Co(NCS)_2(abpt)_2$ did not show any evidence of a thermally-induced spin crossover for either of the polymorphs between 300 (2) and 120 (2) K.

Acknowledgements

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supporting information

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$Co(NCS)_2(abpt)_2$ and $Ni(NCS)_2(abpt)_2$ [abpt is 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole]: structural characterization of polymorphs A and B

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Computing details

Data collection: *SMART* (Bruker, 1999) for Co_A_120K, Co_B_120K, Ni_B_120K, Co_A_300K, Co_B_300K; *APEX2* (Bruker, 2005) for Ni_A_120K. Cell refinement: *SAINT* (Bruker, 2003) for Co_A_120K, Co_B_120K, Ni_B_120K, Co_A_300K, Co_B_300K; *APEX2* (Bruker, 2005) for Ni_A_120K. Data reduction: *SAINT* (Bruker, 2003) for Co_A_120K, Co_B_120K, Ni_B_120K, Co_A_300K, Co_B_300K; *SAINT-Plus* (Bruker, 2013) for Ni_A_120K. For all structures, program(s) used to solve structure: *SHELXS* (Sheldrick, 2008). Program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015) for Co_A_120K, Co_B_120K, Ni_A_120K, Ni_B_120K, Co_A_300K; *SHELXL2014* (Sheldrick, 2015) for Co_B_300K. For all structures, molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)cobalt(II) (Co_A_120K)

Crystal data

$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$
$M_r = 651.61$
Monoclinic, $P2_1/n$
$a = 8.4792$ (6) Å
$b = 10.1307$ (7) Å
$c = 16.3774$ (11) Å
$\beta = 93.485$ (1)°
$V = 1404.22$ (17) Å^3
$Z = 2$
$F(000) = 666$
$D_x = 1.541$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6392 reflections
$\theta = 2.4$–$28.4°$
$\mu = 0.81$ mm^{-1}
$T = 120$ K
Block, orange
0.24 × 0.16 × 0.11 mm

Data collection

Bruker SMART CCD 1K area detector diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
$T_{min} = 0.793$, $T_{max} = 0.919$
13341 measured reflections
2884 independent reflections
2383 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.093$
$S = 1.06$
2884 reflections

202 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 1.6189P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.500000	0.500000	0.500000	0.01882 (13)
S1	0.26353 (8)	0.71891 (7)	0.25547 (4)	0.03309 (19)
N1	0.3933 (2)	0.5708 (2)	0.38833 (13)	0.0251 (5)
N2	0.7191 (2)	0.5974 (2)	0.47456 (12)	0.0229 (5)
N3	0.4751 (2)	0.6892 (2)	0.54812 (13)	0.0252 (5)
N4	0.3563 (2)	0.7585 (2)	0.58160 (12)	0.0212 (4)
N5	0.5684 (2)	0.8849 (2)	0.57976 (13)	0.0245 (5)
N6	0.6795 (3)	0.9902 (2)	0.59404 (15)	0.0300 (5)
H6A	0.729 (3)	0.965 (3)	0.6428 (13)	0.036*
H6B	0.623 (4)	1.062 (3)	0.6070 (18)	0.036*
N7	0.3920 (3)	1.0989 (2)	0.64769 (13)	0.0265 (5)
C1	0.3384 (3)	0.6316 (2)	0.33321 (15)	0.0220 (5)
C2	0.8335 (3)	0.5446 (3)	0.43168 (16)	0.0260 (6)
H2	0.816515	0.460189	0.407395	0.031*
C3	0.9764 (3)	0.6089 (3)	0.42150 (17)	0.0294 (6)
H3	1.054378	0.569724	0.389995	0.035*
C4	1.0025 (3)	0.7307 (3)	0.45807 (17)	0.0320 (6)
H4	1.099888	0.775451	0.452950	0.038*
C5	0.8846 (3)	0.7871 (3)	0.50249 (16)	0.0279 (6)
H5	0.900354	0.870360	0.528377	0.033*
C6	0.7438 (3)	0.7189 (3)	0.50807 (15)	0.0238 (5)
C7	0.6017 (3)	0.7659 (3)	0.54623 (15)	0.0238 (5)
C8	0.4140 (3)	0.8759 (3)	0.60107 (15)	0.0234 (5)
C9	0.3236 (3)	0.9796 (2)	0.64092 (15)	0.0242 (5)
C10	0.3130 (3)	1.1925 (3)	0.68644 (16)	0.0303 (6)
H10	0.359647	1.277459	0.692737	0.036*
C11	0.1660 (3)	1.1714 (3)	0.71792 (16)	0.0286 (6)
H11	0.115389	1.240223	0.745801	0.034*
C12	0.0949 (3)	1.0493 (3)	0.70808 (16)	0.0288 (6)
H12	−0.006542	1.033270	0.727696	0.035*
C13	0.1757 (3)	0.9496 (3)	0.66852 (15)	0.0263 (6)
H13	0.130906	0.864169	0.660766	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0144 (2)	0.0185 (2)	0.0237 (2)	−0.00017 (19)	0.00195 (17)	0.00061 (19)
S1	0.0313 (4)	0.0345 (4)	0.0324 (4)	0.0062 (3)	−0.0072 (3)	0.0043 (3)
N1	0.0206 (11)	0.0265 (12)	0.0283 (11)	−0.0003 (9)	0.0016 (9)	0.0013 (9)
N2	0.0171 (10)	0.0242 (11)	0.0271 (11)	0.0009 (9)	−0.0003 (8)	0.0040 (9)
N3	0.0205 (11)	0.0264 (12)	0.0289 (11)	0.0008 (9)	0.0030 (9)	0.0014 (9)
N4	0.0170 (10)	0.0202 (11)	0.0264 (11)	0.0007 (8)	0.0014 (8)	0.0001 (8)
N5	0.0219 (11)	0.0228 (11)	0.0286 (11)	−0.0052 (9)	0.0002 (9)	−0.0010 (9)
N6	0.0246 (12)	0.0260 (12)	0.0391 (13)	−0.0069 (10)	−0.0004 (10)	−0.0006 (11)
N7	0.0254 (12)	0.0240 (12)	0.0301 (11)	−0.0018 (10)	0.0004 (9)	−0.0014 (9)
C1	0.0154 (12)	0.0234 (13)	0.0277 (13)	−0.0019 (10)	0.0045 (10)	−0.0036 (11)
C2	0.0205 (13)	0.0245 (13)	0.0332 (14)	0.0040 (11)	0.0017 (10)	0.0046 (11)
C3	0.0195 (13)	0.0306 (15)	0.0386 (15)	0.0045 (11)	0.0062 (11)	0.0060 (12)
C4	0.0185 (13)	0.0367 (16)	0.0409 (16)	−0.0031 (12)	0.0021 (11)	0.0082 (13)
C5	0.0229 (13)	0.0303 (14)	0.0301 (13)	−0.0040 (12)	−0.0009 (10)	0.0019 (11)
C6	0.0178 (12)	0.0268 (13)	0.0264 (13)	−0.0001 (11)	−0.0008 (10)	0.0053 (11)
C7	0.0214 (13)	0.0235 (13)	0.0263 (13)	−0.0037 (11)	−0.0010 (10)	0.0019 (10)
C8	0.0205 (13)	0.0264 (14)	0.0232 (12)	−0.0010 (11)	−0.0003 (10)	0.0022 (10)
C9	0.0244 (13)	0.0209 (13)	0.0268 (13)	0.0021 (10)	−0.0013 (10)	0.0035 (10)
C10	0.0313 (15)	0.0273 (15)	0.0322 (14)	−0.0013 (12)	0.0003 (12)	−0.0064 (11)
C11	0.0301 (15)	0.0287 (14)	0.0270 (14)	0.0029 (12)	0.0029 (11)	−0.0054 (11)
C12	0.0307 (15)	0.0293 (14)	0.0268 (13)	−0.0011 (12)	0.0040 (11)	0.0032 (11)
C13	0.0277 (14)	0.0223 (13)	0.0284 (13)	−0.0030 (11)	−0.0021 (11)	0.0030 (11)

Geometric parameters (Å, º)

Co1—N1	2.116 (2)	N7—C10	1.342 (3)
Co1—N1^{i}	2.116 (2)	C2—H2	0.9500
Co1—N2^{i}	2.166 (2)	C2—C3	1.394 (4)
Co1—N2	2.166 (2)	C3—H3	0.9500
Co1—N3	2.088 (2)	C3—C4	1.384 (4)
Co1—N3^{i}	2.088 (2)	C4—H4	0.9500
S1—C1	1.646 (3)	C4—C5	1.394 (4)
N1—C1	1.166 (3)	C5—H5	0.9500
N2—C2	1.343 (3)	C5—C6	1.388 (4)
N2—C6	1.358 (3)	C6—C7	1.470 (4)
N3—N4	1.370 (3)	C8—C9	1.475 (4)
N3—C7	1.327 (3)	C9—C13	1.393 (4)
N4—C8	1.318 (3)	C10—H10	0.9500
N5—N6	1.433 (3)	C10—C11	1.394 (4)
N5—C7	1.361 (3)	C11—H11	0.9500
N5—C8	1.378 (3)	C11—C12	1.382 (4)
N6—H6A	0.915 (18)	C12—H12	0.9500
N6—H6B	0.90 (3)	C12—C13	1.401 (4)
N7—C9	1.343 (3)	C13—H13	0.9500

N1—Co1—N1^{i}	180.00 (11)	C2—C3—H3	120.6
N1—Co1—N2^{i}	89.66 (8)	C4—C3—C2	118.9 (3)
N1^{i}—Co1—N2^{i}	90.34 (8)	C4—C3—H3	120.6
N1^{i}—Co1—N2	89.66 (8)	C3—C4—H4	120.3
N1—Co1—N2	90.34 (8)	C3—C4—C5	119.3 (3)
N2—Co1—N2^{i}	180.0	C5—C4—H4	120.3
N3^{i}—Co1—N1	91.88 (8)	C4—C5—H5	120.7
N3^{i}—Co1—N1^{i}	88.12 (8)	C6—C5—C4	118.5 (3)
N3—Co1—N1^{i}	91.88 (8)	C6—C5—H5	120.7
N3—Co1—N1	88.12 (8)	N2—C6—C5	122.4 (2)
N3—Co1—N2	76.22 (8)	N2—C6—C7	110.8 (2)
N3^{i}—Co1—N2^{i}	76.22 (8)	C5—C6—C7	126.7 (2)
N3^{i}—Co1—N2	103.78 (8)	N3—C7—N5	108.8 (2)
N3—Co1—N2^{i}	103.78 (8)	N3—C7—C6	120.3 (2)
N3—Co1—N3^{i}	180.0	N5—C7—C6	130.9 (2)
C1—N1—Co1	167.9 (2)	N4—C8—N5	110.0 (2)
C2—N2—Co1	125.03 (18)	N4—C8—C9	123.6 (2)
C2—N2—C6	118.3 (2)	N5—C8—C9	126.3 (2)
C6—N2—Co1	116.60 (16)	N7—C9—C8	116.4 (2)
N4—N3—Co1	135.68 (16)	N7—C9—C13	124.2 (2)
C7—N3—Co1	115.38 (17)	C13—C9—C8	119.4 (2)
C7—N3—N4	108.9 (2)	N7—C10—H10	118.3
C8—N4—N3	106.8 (2)	N7—C10—C11	123.4 (3)
C7—N5—N6	125.1 (2)	C11—C10—H10	118.3
C7—N5—C8	105.5 (2)	C10—C11—H11	120.4
C8—N5—N6	129.2 (2)	C12—C11—C10	119.2 (3)
N5—N6—H6A	101 (2)	C12—C11—H11	120.4
N5—N6—H6B	107 (2)	C11—C12—H12	120.7
H6A—N6—H6B	104 (3)	C11—C12—C13	118.5 (3)
C10—N7—C9	116.7 (2)	C13—C12—H12	120.7
N1—C1—S1	179.1 (2)	C9—C13—C12	117.9 (2)
N2—C2—H2	118.8	C9—C13—H13	121.0
N2—C2—C3	122.4 (3)	C12—C13—H13	121.0
C3—C2—H2	118.8		

Co1—N2—C2—C3	−175.97 (19)	N7—C10—C11—C12	−1.2 (4)
Co1—N2—C6—C5	174.34 (19)	C2—N2—C6—C5	−2.8 (4)
Co1—N2—C6—C7	−7.9 (3)	C2—N2—C6—C7	175.0 (2)
Co1—N3—N4—C8	179.89 (18)	C2—C3—C4—C5	−1.4 (4)
Co1—N3—C7—N5	−179.68 (15)	C3—C4—C5—C6	−0.4 (4)
Co1—N3—C7—C6	3.2 (3)	C4—C5—C6—N2	2.6 (4)
N2—C2—C3—C4	1.2 (4)	C4—C5—C6—C7	−174.8 (2)
N2—C6—C7—N3	3.2 (3)	C5—C6—C7—N3	−179.1 (2)
N2—C6—C7—N5	−173.2 (2)	C5—C6—C7—N5	4.5 (4)
N3—N4—C8—N5	0.8 (3)	C6—N2—C2—C3	0.9 (4)
N3—N4—C8—C9	−178.4 (2)	C7—N3—N4—C8	−1.2 (3)
N4—N3—C7—N5	1.2 (3)	C7—N5—C8—N4	−0.1 (3)
N4—N3—C7—C6	−175.9 (2)	C7—N5—C8—C9	179.1 (2)

N4—C8—C9—N7	−172.1 (2)	C8—N5—C7—N3	−0.7 (3)
N4—C8—C9—C13	7.6 (4)	C8—N5—C7—C6	176.0 (3)
N5—C8—C9—N7	8.8 (4)	C8—C9—C13—C12	178.3 (2)
N5—C8—C9—C13	−171.4 (2)	C9—N7—C10—C11	−0.9 (4)
N6—N5—C7—N3	175.1 (2)	C10—N7—C9—C8	−177.7 (2)
N6—N5—C7—C6	−8.2 (4)	C10—N7—C9—C13	2.5 (4)
N6—N5—C8—N4	−175.6 (2)	C10—C11—C12—C13	1.7 (4)
N6—N5—C8—C9	3.5 (4)	C11—C12—C13—C9	−0.3 (4)
N7—C9—C13—C12	−2.0 (4)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*B*···N7	0.90 (3)	2.14 (3)	2.861 (3)	136 (3)
C5—H5···N6	0.95	2.53	3.135 (4)	122

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)cobalt(II) (Co_B_120K)

Crystal data

$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r = 651.61
Monoclinic, $P2_1/n$
a = 11.4978 (5) Å
b = 9.5235 (4) Å
c = 12.7179 (5) Å
β = 100.771 (1)°
V = 1368.07 (10) Å^3
Z = 2
$F(000)$ = 666
D_x = 1.582 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7088 reflections
θ = 2.7–28.3°
μ = 0.83 mm^{-1}
T = 120 K
Block, yellow
0.48 × 0.22 × 0.1 mm

Data collection

CCD area detector diffractometer
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.755, T_{max} = 0.884
13084 measured reflections
2799 independent reflections
2363 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 26.4°, θ_{min} = 2.2°
h = −14→14
k = −11→11
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.065
S = 1.03
2799 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0223P)^2 + 0.9469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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}
Co1	0.500000	0.500000	0.500000	0.01662 (10)
S1	0.47702 (4)	0.70612 (5)	0.14549 (4)	0.02147 (12)
N1	0.51090 (14)	0.58552 (17)	0.35006 (12)	0.0226 (3)
N2	0.54062 (13)	0.70429 (16)	0.57154 (11)	0.0184 (3)
N3	0.33257 (12)	0.59797 (16)	0.48313 (11)	0.0185 (3)
N4	0.21930 (13)	0.56657 (16)	0.43186 (12)	0.0190 (3)
N5	0.22659 (12)	0.78694 (15)	0.48602 (11)	0.0164 (3)
N6	0.19418 (14)	0.92348 (16)	0.51462 (14)	0.0212 (3)
H6A	0.1431 (18)	0.911 (2)	0.5580 (16)	0.025*
H6B	0.1556 (18)	0.963 (2)	0.4536 (18)	0.025*
N7	−0.00410 (13)	0.82632 (16)	0.35394 (12)	0.0207 (3)
C1	0.49638 (15)	0.63560 (19)	0.26536 (14)	0.0180 (4)
C2	0.64830 (16)	0.7492 (2)	0.61788 (14)	0.0215 (4)
H2	0.713997	0.688352	0.619097	0.026*
C3	0.66794 (16)	0.8809 (2)	0.66415 (14)	0.0232 (4)
H3	0.745571	0.909506	0.696411	0.028*
C4	0.57273 (16)	0.9697 (2)	0.66257 (15)	0.0234 (4)
H4	0.583973	1.059817	0.694983	0.028*
C5	0.46048 (16)	0.9265 (2)	0.61328 (14)	0.0204 (4)
H5	0.394057	0.986769	0.609838	0.024*
C6	0.44783 (15)	0.79323 (19)	0.56929 (13)	0.0175 (4)
C7	0.33619 (15)	0.72999 (19)	0.51515 (13)	0.0167 (4)
C8	0.15649 (15)	0.68144 (19)	0.43460 (14)	0.0175 (4)
C9	0.02990 (15)	0.69740 (18)	0.38880 (14)	0.0171 (4)
C10	−0.11930 (16)	0.8441 (2)	0.31474 (15)	0.0242 (4)
H10	−0.144940	0.934109	0.287596	0.029*
C11	−0.20318 (16)	0.7402 (2)	0.31123 (15)	0.0255 (4)
H11	−0.284590	0.759252	0.285291	0.031*
C12	−0.16601 (17)	0.6076 (2)	0.34634 (15)	0.0259 (4)
H12	−0.221505	0.533282	0.344512	0.031*
C13	−0.04681 (16)	0.5844 (2)	0.38420 (14)	0.0221 (4)
H13	−0.018285	0.493504	0.406456	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01448 (17)	0.01855 (18)	0.01672 (17)	0.00225 (14)	0.00261 (13)	0.00024 (14)
S1	0.0220 (2)	0.0208 (2)	0.0215 (2)	0.00129 (19)	0.00387 (18)	0.00472 (18)
N1	0.0232 (8)	0.0235 (9)	0.0219 (8)	0.0013 (7)	0.0058 (7)	0.0004 (7)

N2	0.0165 (7)	0.0221 (8)	0.0163 (7)	0.0003 (6)	0.0029 (6)	0.0009 (6)
N3	0.0153 (7)	0.0204 (8)	0.0191 (7)	0.0000 (6)	0.0016 (6)	−0.0007 (6)
N4	0.0146 (7)	0.0208 (8)	0.0208 (8)	0.0017 (6)	0.0011 (6)	−0.0003 (6)
N5	0.0140 (7)	0.0164 (7)	0.0187 (7)	0.0010 (6)	0.0034 (6)	−0.0006 (6)
N6	0.0194 (8)	0.0170 (8)	0.0270 (9)	0.0034 (6)	0.0040 (7)	−0.0032 (7)
N7	0.0184 (8)	0.0197 (8)	0.0224 (8)	−0.0009 (6)	−0.0002 (6)	0.0012 (6)
C1	0.0135 (8)	0.0174 (9)	0.0235 (10)	−0.0003 (7)	0.0046 (7)	−0.0028 (8)
C2	0.0163 (9)	0.0267 (10)	0.0213 (9)	0.0015 (8)	0.0036 (7)	0.0004 (8)
C3	0.0196 (9)	0.0286 (11)	0.0210 (9)	−0.0035 (8)	0.0026 (8)	−0.0013 (8)
C4	0.0242 (10)	0.0248 (10)	0.0210 (9)	−0.0035 (8)	0.0038 (8)	−0.0045 (8)
C5	0.0190 (9)	0.0210 (10)	0.0214 (9)	0.0018 (7)	0.0044 (7)	−0.0010 (7)
C6	0.0163 (9)	0.0221 (9)	0.0149 (8)	−0.0002 (7)	0.0051 (7)	0.0024 (7)
C7	0.0153 (8)	0.0196 (9)	0.0158 (8)	0.0020 (7)	0.0047 (7)	0.0018 (7)
C8	0.0155 (9)	0.0202 (9)	0.0171 (8)	−0.0003 (7)	0.0035 (7)	0.0007 (7)
C9	0.0167 (9)	0.0183 (9)	0.0164 (8)	0.0012 (7)	0.0031 (7)	−0.0010 (7)
C10	0.0202 (9)	0.0232 (10)	0.0276 (10)	0.0046 (8)	0.0004 (8)	0.0015 (8)
C11	0.0159 (9)	0.0338 (11)	0.0258 (10)	0.0000 (8)	0.0016 (8)	−0.0008 (8)
C12	0.0227 (10)	0.0294 (11)	0.0241 (10)	−0.0103 (8)	0.0003 (8)	−0.0009 (8)
C13	0.0247 (10)	0.0192 (9)	0.0210 (9)	−0.0015 (8)	0.0003 (8)	−0.0003 (7)

Geometric parameters (Å, º)

Co1—N1	2.0987 (15)	N7—C10	1.336 (2)
Co1—N1^{i}	2.0987 (15)	C2—H2	0.9500
Co1—N2^{i}	2.1616 (15)	C2—C3	1.385 (3)
Co1—N2	2.1616 (15)	C3—H3	0.9500
Co1—N3^{i}	2.1137 (14)	C3—C4	1.381 (3)
Co1—N3	2.1138 (14)	C4—H4	0.9500
S1—C1	1.6425 (18)	C4—C5	1.388 (3)
N1—C1	1.161 (2)	C5—H5	0.9500
N2—C2	1.338 (2)	C5—C6	1.383 (3)
N2—C6	1.358 (2)	C6—C7	1.468 (2)
N3—N4	1.376 (2)	C8—C9	1.471 (2)
N3—C7	1.320 (2)	C9—C13	1.386 (3)
N4—C8	1.315 (2)	C10—H10	0.9500
N5—N6	1.419 (2)	C10—C11	1.377 (3)
N5—C7	1.358 (2)	C11—H11	0.9500
N5—C8	1.375 (2)	C11—C12	1.381 (3)
N6—H6A	0.89 (2)	C12—H12	0.9500
N6—H6B	0.90 (2)	C12—C13	1.383 (3)
N7—C9	1.339 (2)	C13—H13	0.9500
N1—Co1—N1^{i}	180.0	C2—C3—H3	120.6
N1—Co1—N2	89.33 (6)	C4—C3—C2	118.86 (17)
N1—Co1—N2^{i}	90.67 (6)	C4—C3—H3	120.6
N1^{i}—Co1—N2	90.67 (6)	C3—C4—H4	120.3
N1^{i}—Co1—N2^{i}	89.33 (6)	C3—C4—C5	119.49 (18)
N1—Co1—N3^{i}	93.19 (6)	C5—C4—H4	120.3

N1—Co1—N3	86.81 (6)	C4—C5—H5	120.9
N1^{i}—Co1—N3	93.19 (6)	C6—C5—C4	118.27 (17)
N1^{i}—Co1—N3^{i}	86.81 (6)	C6—C5—H5	120.9
N2—Co1—N2^{i}	180.0	N2—C6—C5	122.73 (16)
N3^{i}—Co1—N2^{i}	76.49 (6)	N2—C6—C7	111.63 (15)
N3—Co1—N2^{i}	103.50 (6)	C5—C6—C7	125.64 (16)
N3^{i}—Co1—N2	103.50 (6)	N3—C7—N5	108.79 (15)
N3—Co1—N2	76.50 (6)	N3—C7—C6	120.67 (15)
N3^{i}—Co1—N3	180.0	N5—C7—C6	130.51 (16)
C1—N1—Co1	168.40 (14)	N4—C8—N5	110.16 (15)
C2—N2—Co1	125.63 (12)	N4—C8—C9	125.67 (16)
C2—N2—C6	117.92 (16)	N5—C8—C9	124.16 (16)
C6—N2—Co1	116.44 (11)	N7—C9—C8	115.60 (15)
N4—N3—Co1	135.69 (11)	N7—C9—C13	123.64 (16)
C7—N3—Co1	114.43 (11)	C13—C9—C8	120.76 (16)
C7—N3—N4	109.01 (14)	N7—C10—H10	118.0
C8—N4—N3	106.41 (14)	N7—C10—C11	124.09 (18)
C7—N5—N6	124.80 (15)	C11—C10—H10	118.0
C7—N5—C8	105.63 (14)	C10—C11—H11	120.8
C8—N5—N6	129.29 (14)	C10—C11—C12	118.33 (17)
N5—N6—H6A	105.7 (14)	C12—C11—H11	120.8
N5—N6—H6B	105.8 (13)	C11—C12—H12	120.5
H6A—N6—H6B	108.4 (19)	C11—C12—C13	119.03 (18)
C10—N7—C9	116.60 (16)	C13—C12—H12	120.5
N1—C1—S1	179.51 (17)	C9—C13—H13	120.9
N2—C2—H2	118.6	C12—C13—C9	118.20 (18)
N2—C2—C3	122.71 (17)	C12—C13—H13	120.9
C3—C2—H2	118.6		

Co1—N2—C2—C3	−178.73 (13)	N7—C10—C11—C12	−2.7 (3)
Co1—N2—C6—C5	179.12 (13)	C2—N2—C6—C5	−0.5 (2)
Co1—N2—C6—C7	−1.01 (18)	C2—N2—C6—C7	179.41 (15)
Co1—N3—N4—C8	−168.52 (13)	C2—C3—C4—C5	−1.1 (3)
Co1—N3—C7—N5	171.13 (10)	C3—C4—C5—C6	1.5 (3)
Co1—N3—C7—C6	−6.9 (2)	C4—C5—C6—N2	−0.7 (3)
N2—C2—C3—C4	0.0 (3)	C4—C5—C6—C7	179.48 (16)
N2—C6—C7—N3	5.3 (2)	C5—C6—C7—N3	−174.83 (16)
N2—C6—C7—N5	−172.26 (16)	C5—C6—C7—N5	7.6 (3)
N3—N4—C8—N5	0.31 (19)	C6—N2—C2—C3	0.8 (3)
N3—N4—C8—C9	179.70 (15)	C7—N3—N4—C8	−0.27 (19)
N4—N3—C7—N5	0.12 (19)	C7—N5—C8—N4	−0.24 (19)
N4—N3—C7—C6	−177.92 (14)	C7—N5—C8—C9	−179.64 (16)
N4—C8—C9—N7	−149.33 (17)	C8—N5—C7—N3	0.06 (18)
N4—C8—C9—C13	31.2 (3)	C8—N5—C7—C6	177.85 (17)
N5—C8—C9—N7	30.0 (2)	C8—C9—C13—C12	176.13 (16)
N5—C8—C9—C13	−149.47 (17)	C9—N7—C10—C11	1.8 (3)
N6—N5—C7—N3	174.49 (15)	C10—N7—C9—C8	−178.21 (15)
N6—N5—C7—C6	−7.7 (3)	C10—N7—C9—C13	1.2 (3)

N6—N5—C8—N4	−174.33 (16)	C10—C11—C12—C13	0.5 (3)
N6—N5—C8—C9	6.3 (3)	C11—C12—C13—C9	2.3 (3)
N7—C9—C13—C12	−3.3 (3)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···S1^{ii}	0.89 (2)	2.63 (2)	3.4758 (17)	159.9 (18)
N6—H6*B*···N7	0.90 (2)	2.41 (2)	2.914 (2)	115.6 (16)
C5—H5···N6	0.95	2.46	3.084 (2)	123

Symmetry code: (ii) *x*−1/2, −*y*+3/2, *z*+1/2.

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)nickel(II) (Ni_A_120K)

Crystal data

$[Ni(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r = 651.39
Monoclinic, $P2_1/n$
a = 8.4041 (7) Å
b = 10.0681 (9) Å
c = 16.2360 (14) Å
β = 93.060 (2)°
V = 1371.8 (2) Å^3
Z = 2
$F(000)$ = 668
D_x = 1.577 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5417 reflections
θ = 2.4–28.3°
μ = 0.91 mm^{-1}
T = 120 K
Block, violet
0.2 × 0.12 × 0.08 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.781, T_{max} = 0.936
15450 measured reflections
2819 independent reflections
2161 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 26.4°, θ_{min} = 2.4°
h = −10→10
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.085
S = 1.02
2819 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.9816P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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	0.500000	0.500000	0.500000	0.01868 (13)
S1	0.26497 (8)	0.71955 (7)	0.25670 (4)	0.03080 (18)
N1	0.3946 (2)	0.5705 (2)	0.38980 (13)	0.0232 (5)
N2	0.7167 (2)	0.5919 (2)	0.47342 (12)	0.0215 (5)
N3	0.4739 (2)	0.6856 (2)	0.54834 (12)	0.0227 (5)
N4	0.3551 (2)	0.7556 (2)	0.58167 (12)	0.0206 (5)
N5	0.5684 (2)	0.8809 (2)	0.57977 (12)	0.0221 (5)
N6	0.6807 (3)	0.9858 (2)	0.59360 (15)	0.0283 (5)
H6A	0.736 (3)	0.958 (3)	0.6456 (18)	0.034*
H6B	0.626 (3)	1.057 (3)	0.6073 (17)	0.034*
N7	0.3922 (2)	1.0973 (2)	0.64693 (13)	0.0245 (5)
C1	0.3403 (3)	0.6317 (2)	0.33474 (16)	0.0213 (5)
C2	0.8299 (3)	0.5388 (3)	0.42949 (16)	0.0238 (6)
H2	0.811395	0.454460	0.404488	0.029*
C3	0.9737 (3)	0.6021 (3)	0.41898 (16)	0.0266 (6)
H3	1.051516	0.562634	0.386381	0.032*
C4	1.0023 (3)	0.7228 (3)	0.45632 (16)	0.0281 (6)
H4	1.101367	0.766657	0.450993	0.034*
C5	0.8857 (3)	0.7800 (3)	0.50177 (16)	0.0252 (6)
H5	0.903075	0.863283	0.528222	0.030*
C6	0.7435 (3)	0.7131 (3)	0.50774 (15)	0.0221 (5)
C7	0.6016 (3)	0.7616 (2)	0.54657 (15)	0.0216 (5)
C8	0.4127 (3)	0.8732 (3)	0.60082 (15)	0.0223 (5)
C9	0.3233 (3)	0.9779 (2)	0.64037 (15)	0.0223 (6)
C13	0.3135 (3)	1.1913 (3)	0.68588 (16)	0.0264 (6)
H13	0.361618	1.276291	0.692325	0.032*
C12	0.1651 (3)	1.1718 (3)	0.71752 (15)	0.0256 (6)
H12	0.113952	1.241427	0.745448	0.031*
C11	0.0934 (3)	1.0491 (3)	0.70755 (16)	0.0266 (6)
H11	−0.009382	1.033503	0.727210	0.032*
C10	0.1735 (3)	0.9489 (3)	0.66848 (16)	0.0247 (6)
H10	0.127702	0.863226	0.661092	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0143 (2)	0.0209 (2)	0.0211 (2)	−0.00047 (19)	0.00328 (17)	0.0002 (2)
S1	0.0281 (4)	0.0350 (4)	0.0286 (4)	0.0053 (3)	−0.0039 (3)	0.0032 (3)
N1	0.0168 (10)	0.0280 (12)	0.0248 (11)	0.0015 (9)	0.0026 (9)	0.0006 (10)

N2	0.0163 (10)	0.0246 (12)	0.0237 (11)	0.0007 (9)	0.0015 (9)	0.0044 (9)
N3	0.0175 (10)	0.0265 (12)	0.0240 (11)	−0.0009 (9)	0.0016 (9)	−0.0011 (9)
N4	0.0172 (10)	0.0211 (12)	0.0235 (11)	0.0011 (8)	0.0022 (9)	−0.0014 (9)
N5	0.0192 (10)	0.0237 (12)	0.0234 (11)	−0.0026 (9)	0.0012 (9)	0.0004 (9)
N6	0.0215 (11)	0.0277 (13)	0.0355 (13)	−0.0071 (10)	0.0006 (10)	−0.0037 (11)
N7	0.0232 (11)	0.0240 (12)	0.0264 (11)	−0.0014 (9)	0.0023 (9)	−0.0020 (10)
C1	0.0147 (12)	0.0232 (13)	0.0266 (14)	−0.0013 (10)	0.0055 (11)	−0.0055 (11)
C2	0.0201 (12)	0.0258 (14)	0.0256 (13)	0.0042 (10)	0.0011 (11)	0.0037 (11)
C3	0.0177 (12)	0.0316 (15)	0.0306 (15)	0.0038 (11)	0.0038 (11)	0.0067 (12)
C4	0.0170 (12)	0.0339 (15)	0.0333 (15)	−0.0021 (11)	0.0018 (11)	0.0070 (13)
C5	0.0194 (12)	0.0288 (14)	0.0274 (14)	−0.0038 (11)	−0.0001 (11)	0.0011 (12)
C6	0.0179 (12)	0.0257 (14)	0.0225 (13)	0.0003 (11)	−0.0010 (10)	0.0041 (11)
C7	0.0203 (12)	0.0244 (14)	0.0200 (12)	−0.0012 (11)	0.0003 (10)	0.0017 (10)
C8	0.0200 (12)	0.0282 (14)	0.0188 (12)	−0.0004 (11)	0.0009 (10)	0.0034 (11)
C9	0.0233 (12)	0.0216 (14)	0.0217 (13)	0.0007 (10)	−0.0003 (10)	0.0021 (10)
C13	0.0252 (13)	0.0273 (15)	0.0266 (14)	−0.0020 (11)	0.0008 (11)	−0.0047 (12)
C12	0.0279 (13)	0.0268 (14)	0.0223 (14)	0.0026 (11)	0.0022 (11)	−0.0030 (11)
C11	0.0252 (13)	0.0298 (14)	0.0252 (14)	−0.0015 (12)	0.0046 (11)	0.0043 (12)
C10	0.0262 (13)	0.0221 (13)	0.0255 (13)	−0.0025 (11)	−0.0007 (11)	0.0023 (11)

Geometric parameters (Å, º)

Ni1—N1^{i}	2.079 (2)	N7—C13	1.333 (3)
Ni1—N1	2.079 (2)	C2—H2	0.9500
Ni1—N2	2.1076 (19)	C2—C3	1.386 (3)
Ni1—N2^{i}	2.1076 (19)	C3—H3	0.9500
Ni1—N3	2.043 (2)	C3—C4	1.373 (4)
Ni1—N3^{i}	2.043 (2)	C4—H4	0.9500
S1—C1	1.644 (3)	C4—C5	1.384 (4)
N1—C1	1.159 (3)	C5—H5	0.9500
N2—C2	1.331 (3)	C5—C6	1.380 (3)
N2—C6	1.356 (3)	C6—C7	1.462 (3)
N3—N4	1.358 (3)	C8—C9	1.463 (3)
N3—C7	1.320 (3)	C9—C10	1.392 (3)
N4—C8	1.310 (3)	C13—H13	0.9500
N5—N6	1.426 (3)	C13—C12	1.388 (4)
N5—C7	1.352 (3)	C12—H12	0.9500
N5—C8	1.373 (3)	C12—C11	1.381 (4)
N6—H6A	0.98 (3)	C11—H11	0.9500
N6—H6B	0.88 (3)	C11—C10	1.384 (4)
N7—C9	1.337 (3)	C10—H10	0.9500
N1^{i}—Ni1—N1	180.0	C2—C3—H3	120.4
N1—Ni1—N2^{i}	89.60 (8)	C4—C3—C2	119.1 (2)
N1^{i}—Ni1—N2	89.60 (8)	C4—C3—H3	120.4
N1—Ni1—N2	90.40 (8)	C3—C4—H4	120.3
N1^{i}—Ni1—N2^{i}	90.40 (8)	C3—C4—C5	119.4 (2)
N2^{i}—Ni1—N2	180.0	C5—C4—H4	120.3

N3—Ni1—N1	88.21 (8)	C4—C5—H5	120.8
N3—Ni1—N1^{i}	91.79 (8)	C6—C5—C4	118.4 (2)
N3^{i}—Ni1—N1^{i}	88.21 (8)	C6—C5—H5	120.8
N3^{i}—Ni1—N1	91.79 (8)	N2—C6—C5	122.4 (2)
N3—Ni1—N2^{i}	102.19 (8)	N2—C6—C7	110.9 (2)
N3^{i}—Ni1—N2^{i}	77.81 (8)	C5—C6—C7	126.6 (2)
N3—Ni1—N2	77.81 (8)	N3—C7—N5	108.7 (2)
N3^{i}—Ni1—N2	102.19 (8)	N3—C7—C6	119.9 (2)
N3—Ni1—N3^{i}	180.0	N5—C7—C6	131.2 (2)
C1—N1—Ni1	167.9 (2)	N4—C8—N5	109.7 (2)
C2—N2—Ni1	125.68 (18)	N4—C8—C9	124.3 (2)
C2—N2—C6	118.3 (2)	N5—C8—C9	126.0 (2)
C6—N2—Ni1	115.94 (16)	N7—C9—C8	116.9 (2)
N4—N3—Ni1	136.40 (16)	N7—C9—C10	123.9 (2)
C7—N3—Ni1	114.70 (16)	C10—C9—C8	119.2 (2)
C7—N3—N4	108.9 (2)	N7—C13—H13	118.2
C8—N4—N3	107.07 (19)	N7—C13—C12	123.6 (2)
C7—N5—N6	124.9 (2)	C12—C13—H13	118.2
C7—N5—C8	105.6 (2)	C13—C12—H12	120.7
C8—N5—N6	129.4 (2)	C11—C12—C13	118.6 (2)
N5—N6—H6A	101.7 (17)	C11—C12—H12	120.7
N5—N6—H6B	106.7 (19)	C12—C11—H11	120.5
H6A—N6—H6B	104 (2)	C12—C11—C10	119.1 (2)
C13—N7—C9	116.9 (2)	C10—C11—H11	120.5
N1—C1—S1	179.4 (2)	C9—C10—H10	121.0
N2—C2—H2	118.9	C11—C10—C9	117.9 (2)
N2—C2—C3	122.3 (2)	C11—C10—H10	121.0
C3—C2—H2	118.9		

Ni1—N2—C2—C3	−175.85 (18)	N7—C13—C12—C11	−0.8 (4)
Ni1—N2—C6—C5	174.22 (19)	C2—N2—C6—C5	−2.9 (4)
Ni1—N2—C6—C7	−8.4 (3)	C2—N2—C6—C7	174.4 (2)
Ni1—N3—N4—C8	−179.20 (18)	C2—C3—C4—C5	−1.6 (4)
Ni1—N3—C7—N5	179.72 (15)	C3—C4—C5—C6	−0.2 (4)
Ni1—N3—C7—C6	3.4 (3)	C4—C5—C6—N2	2.5 (4)
N2—C2—C3—C4	1.3 (4)	C4—C5—C6—C7	−174.4 (2)
N2—C6—C7—N3	3.5 (3)	C5—C6—C7—N3	−179.3 (2)
N2—C6—C7—N5	−172.0 (2)	C5—C6—C7—N5	5.2 (4)
N3—N4—C8—N5	0.4 (3)	C6—N2—C2—C3	1.0 (4)
N3—N4—C8—C9	−178.4 (2)	C7—N3—N4—C8	−0.8 (3)
N4—N3—C7—N5	0.9 (3)	C7—N5—C8—N4	0.2 (3)
N4—N3—C7—C6	−175.4 (2)	C7—N5—C8—C9	178.9 (2)
N4—C8—C9—N7	−172.2 (2)	C8—N5—C7—N3	−0.7 (3)
N4—C8—C9—C10	7.6 (4)	C8—N5—C7—C6	175.1 (3)
N5—C8—C9—N7	9.2 (4)	C8—C9—C10—C11	178.4 (2)
N5—C8—C9—C10	−171.0 (2)	C9—N7—C13—C12	−1.5 (4)
N6—N5—C7—N3	175.5 (2)	C13—N7—C9—C8	−177.4 (2)
N6—N5—C7—C6	−8.7 (4)	C13—N7—C9—C10	2.8 (4)

N6—N5—C8—N4	−175.7 (2)	C13—C12—C11—C10	1.7 (4)
N6—N5—C8—C9	3.0 (4)	C12—C11—C10—C9	−0.5 (4)
N7—C9—C10—C11	−1.9 (4)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···S1^{ii}	0.98 (3)	2.54 (3)	3.404 (3)	146 (2)
N6—H6*B*···N7	0.88 (3)	2.14 (3)	2.848 (3)	137 (3)
C2—H2···N4^{i}	0.95	2.55	3.347 (3)	141
C5—H5···N6	0.95	2.52	3.124 (4)	122

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, *z*+1/2.

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)nickel(II) (Ni_B_120K)

Crystal data

$[Ni(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r = 651.39
Monoclinic, $P2_1/n$
a = 11.5860 (14) Å
b = 9.5489 (12) Å
c = 12.8132 (16) Å
β = 100.806 (2)°
V = 1392.4 (3) Å^3
Z = 2
$F(000)$ = 668
D_x = 1.554 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2373 reflections
θ = 2.2–25.7°
μ = 0.89 mm^{-1}
T = 120 K
Prism, clear light violet
0.2 × 0.13 × 0.04 mm

Data collection

Bruker SMART CCD 1K area detector diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.746, T_{max} = 0.948
12077 measured reflections
2552 independent reflections
1666 reflections with $I > 2\sigma(I)$
R_{int} = 0.116
θ_{max} = 25.3°, θ_{min} = 2.2°
h = −13→13
k = −11→11
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.136
S = 1.06
2552 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 2.8959P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 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	0.500000	0.500000	0.500000	0.0168 (3)
S1	0.47860 (11)	0.70416 (15)	0.14676 (11)	0.0220 (3)
N1	0.5113 (3)	0.5822 (5)	0.3520 (4)	0.0227 (10)
N2	0.5425 (3)	0.6994 (4)	0.5705 (3)	0.0208 (10)
N3	0.3342 (3)	0.5953 (5)	0.4815 (3)	0.0190 (10)
N4	0.2208 (3)	0.5626 (4)	0.4299 (3)	0.0195 (10)
N5	0.2283 (3)	0.7837 (4)	0.4860 (3)	0.0171 (9)
N6	0.1968 (4)	0.9206 (5)	0.5157 (4)	0.0209 (10)
H6A	0.149 (5)	0.912 (6)	0.557 (4)	0.025*
H6B	0.170 (5)	0.957 (6)	0.456 (5)	0.025*
N7	−0.0044 (4)	0.8256 (4)	0.3548 (4)	0.0245 (11)
C1	0.4981 (4)	0.6330 (5)	0.2662 (4)	0.0176 (11)
C2	0.6509 (4)	0.7460 (6)	0.6167 (4)	0.0235 (12)
H2	0.716363	0.685978	0.616705	0.028*
C3	0.6708 (5)	0.8768 (6)	0.6638 (4)	0.0241 (13)
H3	0.747743	0.904941	0.696617	0.029*
C4	0.5754 (4)	0.9656 (5)	0.6617 (4)	0.0223 (12)
H4	0.586519	1.055540	0.693738	0.027*
C5	0.4632 (4)	0.9227 (6)	0.6125 (4)	0.0227 (12)
H5	0.397440	0.982974	0.609409	0.027*
C6	0.4505 (4)	0.7909 (5)	0.5685 (4)	0.0187 (11)
C7	0.3383 (4)	0.7267 (5)	0.5142 (4)	0.0191 (11)
C8	0.1580 (4)	0.6780 (5)	0.4334 (4)	0.0174 (11)
C9	0.0311 (4)	0.6930 (5)	0.3886 (4)	0.0190 (12)
C13	−0.1184 (4)	0.8423 (6)	0.3164 (4)	0.0245 (13)
H13	−0.144454	0.932317	0.290414	0.029*
C12	−0.2017 (4)	0.7375 (6)	0.3116 (4)	0.0259 (13)
H12	−0.282377	0.756310	0.285121	0.031*
C11	−0.1646 (5)	0.6039 (6)	0.3465 (4)	0.0277 (13)
H11	−0.219834	0.530072	0.345327	0.033*
C10	−0.0454 (4)	0.5804 (5)	0.3831 (4)	0.0225 (12)
H10	−0.017019	0.489329	0.403935	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0117 (4)	0.0160 (5)	0.0217 (5)	0.0020 (4)	0.0005 (4)	−0.0001 (5)
S1	0.0186 (7)	0.0204 (7)	0.0262 (8)	0.0022 (6)	0.0021 (6)	0.0045 (6)
N1	0.011 (2)	0.025 (3)	0.031 (3)	−0.0021 (19)	0.0010 (19)	−0.006 (2)

N2	0.014 (2)	0.023 (3)	0.024 (3)	0.0006 (19)	−0.0003 (18)	0.002 (2)
N3	0.013 (2)	0.020 (2)	0.022 (2)	0.0003 (18)	−0.0021 (18)	−0.001 (2)
N4	0.014 (2)	0.016 (2)	0.026 (3)	−0.0044 (18)	−0.0023 (18)	0.001 (2)
N5	0.013 (2)	0.014 (2)	0.023 (2)	0.0011 (18)	0.0010 (17)	−0.001 (2)
N6	0.019 (2)	0.016 (3)	0.028 (3)	0.004 (2)	0.005 (2)	−0.002 (2)
N7	0.014 (2)	0.017 (3)	0.040 (3)	0.0047 (18)	−0.001 (2)	0.002 (2)
C1	0.011 (2)	0.017 (3)	0.025 (3)	−0.001 (2)	0.004 (2)	−0.001 (2)
C2	0.019 (3)	0.025 (3)	0.025 (3)	0.003 (2)	−0.002 (2)	−0.002 (2)
C3	0.020 (3)	0.024 (3)	0.025 (3)	−0.005 (2)	−0.003 (2)	−0.001 (3)
C4	0.018 (3)	0.018 (3)	0.030 (3)	−0.002 (2)	0.004 (2)	−0.005 (2)
C5	0.016 (3)	0.023 (3)	0.028 (3)	0.000 (2)	0.001 (2)	−0.004 (3)
C6	0.017 (3)	0.019 (3)	0.019 (3)	0.001 (2)	0.000 (2)	−0.003 (2)
C7	0.016 (3)	0.017 (3)	0.023 (3)	0.004 (2)	0.002 (2)	0.002 (2)
C8	0.012 (2)	0.017 (3)	0.022 (3)	0.001 (2)	−0.001 (2)	−0.003 (2)
C9	0.017 (3)	0.018 (3)	0.020 (3)	0.004 (2)	0.000 (2)	−0.001 (2)
C13	0.018 (3)	0.021 (3)	0.033 (3)	0.004 (2)	−0.001 (2)	−0.003 (3)
C12	0.011 (3)	0.032 (3)	0.032 (3)	−0.002 (2)	−0.002 (2)	−0.002 (3)
C11	0.025 (3)	0.028 (3)	0.029 (3)	−0.010 (3)	0.003 (2)	0.005 (3)
C10	0.027 (3)	0.013 (3)	0.025 (3)	0.001 (2)	−0.002 (2)	−0.001 (2)

Geometric parameters (Å, º)

Ni1—N1	2.080 (5)	N7—C13	1.331 (6)
Ni1—N1^{i}	2.080 (5)	C2—H2	0.9500
Ni1—N2^{i}	2.126 (4)	C2—C3	1.388 (7)
Ni1—N2	2.126 (4)	C3—H3	0.9500
Ni1—N3	2.098 (4)	C3—C4	1.390 (7)
Ni1—N3^{i}	2.098 (4)	C4—H4	0.9500
S1—C1	1.651 (5)	C4—C5	1.395 (7)
N1—C1	1.184 (6)	C5—H5	0.9500
N2—C2	1.359 (6)	C5—C6	1.376 (7)
N2—C6	1.375 (6)	C6—C7	1.487 (7)
N3—N4	1.391 (5)	C8—C9	1.482 (7)
N3—C7	1.321 (6)	C9—C10	1.386 (7)
N4—C8	1.325 (6)	C13—H13	0.9500
N5—N6	1.429 (6)	C13—C12	1.383 (7)
N5—C7	1.371 (6)	C12—H12	0.9500
N5—C8	1.389 (6)	C12—C11	1.393 (8)
N6—H6A	0.84 (5)	C11—H11	0.9500
N6—H6B	0.84 (6)	C11—C10	1.392 (7)
N7—C9	1.376 (6)	C10—H10	0.9500
N1—Ni1—N1^{i}	180.0	C2—C3—H3	120.8
N1^{i}—Ni1—N2	89.98 (17)	C2—C3—C4	118.3 (5)
N1—Ni1—N2	90.02 (17)	C4—C3—H3	120.8
N1^{i}—Ni1—N2^{i}	90.02 (17)	C3—C4—H4	120.0
N1—Ni1—N2^{i}	89.98 (17)	C3—C4—C5	120.0 (5)
N1—Ni1—N3	86.93 (16)	C5—C4—H4	120.0

N1—Ni1—N3^{i}	93.07 (16)	C4—C5—H5	120.9
N1^{i}—Ni1—N3^{i}	86.93 (16)	C6—C5—C4	118.2 (5)
N1^{i}—Ni1—N3	93.07 (16)	C6—C5—H5	120.9
N2—Ni1—N2^{i}	180.0	N2—C6—C5	123.4 (5)
N3—Ni1—N2	78.10 (16)	N2—C6—C7	110.7 (4)
N3—Ni1—N2^{i}	101.90 (16)	C5—C6—C7	125.9 (5)
N3^{i}—Ni1—N2	101.90 (16)	N3—C7—N5	108.5 (4)
N3^{i}—Ni1—N2^{i}	78.10 (16)	N3—C7—C6	121.1 (4)
N3—Ni1—N3^{i}	180.0	N5—C7—C6	130.4 (5)
C1—N1—Ni1	168.9 (4)	N4—C8—N5	110.2 (4)
C2—N2—Ni1	126.8 (3)	N4—C8—C9	125.3 (5)
C2—N2—C6	116.8 (4)	N5—C8—C9	124.5 (4)
C6—N2—Ni1	116.4 (3)	N7—C9—C8	115.3 (4)
N4—N3—Ni1	136.0 (3)	N7—C9—C10	123.1 (5)
C7—N3—Ni1	113.5 (3)	C10—C9—C8	121.5 (5)
C7—N3—N4	109.7 (4)	N7—C13—H13	117.8
C8—N4—N3	105.9 (4)	N7—C13—C12	124.4 (5)
C7—N5—N6	124.3 (4)	C12—C13—H13	117.8
C7—N5—C8	105.7 (4)	C13—C12—H12	120.7
C8—N5—N6	129.7 (4)	C13—C12—C11	118.6 (5)
N5—N6—H6A	108 (4)	C11—C12—H12	120.7
N5—N6—H6B	102 (4)	C12—C11—H11	120.6
H6A—N6—H6B	116 (5)	C10—C11—C12	118.8 (5)
C13—N7—C9	116.4 (5)	C10—C11—H11	120.6
N1—C1—S1	179.5 (5)	C9—C10—C11	118.5 (5)
N2—C2—H2	118.4	C9—C10—H10	120.8
N2—C2—C3	123.2 (5)	C11—C10—H10	120.8
C3—C2—H2	118.4		

Ni1—N2—C2—C3	−178.1 (4)	N7—C13—C12—C11	−1.8 (9)
Ni1—N2—C6—C5	178.8 (4)	C2—N2—C6—C5	−1.6 (7)
Ni1—N2—C6—C7	−0.7 (5)	C2—N2—C6—C7	179.0 (4)
Ni1—N3—N4—C8	−169.4 (4)	C2—C3—C4—C5	−0.4 (8)
Ni1—N3—C7—N5	172.2 (3)	C3—C4—C5—C6	1.1 (8)
Ni1—N3—C7—C6	−6.0 (6)	C4—C5—C6—N2	−0.1 (8)
N2—C2—C3—C4	−1.4 (8)	C4—C5—C6—C7	179.3 (5)
N2—C6—C7—N3	4.5 (7)	C5—C6—C7—N3	−175.0 (5)
N2—C6—C7—N5	−173.3 (5)	C5—C6—C7—N5	7.3 (9)
N3—N4—C8—N5	0.0 (6)	C6—N2—C2—C3	2.3 (8)
N3—N4—C8—C9	−179.7 (5)	C7—N3—N4—C8	−0.3 (6)
N4—N3—C7—N5	0.5 (6)	C7—N5—C8—N4	0.3 (6)
N4—N3—C7—C6	−177.7 (4)	C7—N5—C8—C9	180.0 (5)
N4—C8—C9—N7	−150.3 (5)	C8—N5—C7—N3	−0.5 (6)
N4—C8—C9—C10	30.6 (8)	C8—N5—C7—C6	177.5 (5)
N5—C8—C9—N7	30.0 (7)	C8—C9—C10—C11	175.9 (5)
N5—C8—C9—C10	−149.1 (5)	C9—N7—C13—C12	2.1 (8)
N6—N5—C7—N3	174.7 (4)	C13—N7—C9—C8	−178.6 (5)
N6—N5—C7—C6	−7.4 (8)	C13—N7—C9—C10	0.5 (8)

N6—N5—C8—N4	−174.5 (5)	C13—C12—C11—C10	−1.0 (8)
N6—N5—C8—C9	5.2 (8)	C12—C11—C10—C9	3.3 (8)
N7—C9—C10—C11	−3.1 (8)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···S1^{ii}	0.84 (5)	2.70 (5)	3.496 (5)	159 (5)
N6—H6*B*···N7	0.84 (6)	2.52 (5)	2.950 (6)	112 (4)
C2—H2···N4^{i}	0.95	2.59	3.403 (7)	144
C5—H5···N6	0.95	2.48	3.104 (7)	123
C10—H10···S1^{iii}	0.95	2.85	3.710 (5)	151

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1/2, −*y*+3/2, *z*+1/2; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2.

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)cobalt(II) (Co_A_300K)

Crystal data

$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r = 651.61
Monoclinic, $P2_1/n$
a = 8.487 (5) Å
b = 10.249 (6) Å
c = 16.539 (10) Å
β = 93.419 (13)°
V = 1435.9 (14) Å^3
Z = 2
$F(000)$ = 666
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1789 reflections
θ = 2.3–23.5°
μ = 0.79 mm^{-1}
T = 300 K
Block, orange
0.24 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD 1K area detector diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.683, T_{max} = 0.921
7130 measured reflections
2605 independent reflections
1378 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 25.3°, θ_{min} = 2.3°
h = −9→10
k = −11→12
l = −19→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.166
S = 1.02
2605 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.6349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 3 sets of ω scans each set at different φ and/or 2θ angles and each scan (12 s exposure) covering -0.300° degrees in ω. The crystal to detector distance was 4.424 cm.

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	0.500000	0.500000	0.500000	0.0445 (4)
S1	0.26053 (19)	0.71708 (19)	0.25941 (11)	0.0746 (6)
N1	0.3930 (5)	0.5697 (5)	0.3897 (3)	0.0568 (13)
N2	0.7168 (5)	0.5995 (5)	0.4751 (3)	0.0508 (12)
N3	0.4749 (5)	0.6868 (4)	0.5487 (3)	0.0500 (12)
N4	0.3570 (5)	0.7562 (4)	0.5823 (3)	0.0493 (12)
N5	0.5682 (5)	0.8814 (5)	0.5806 (3)	0.0501 (12)
N6	0.6770 (6)	0.9865 (5)	0.5939 (4)	0.0659 (15)
H6A	0.729 (8)	0.971 (6)	0.644 (4)	0.079*
H6B	0.641 (7)	1.063 (6)	0.605 (4)	0.079*
N7	0.3926 (5)	1.0926 (5)	0.6491 (3)	0.0598 (13)
C1	0.3378 (6)	0.6297 (6)	0.3362 (4)	0.0508 (15)
C2	0.8306 (6)	0.5461 (6)	0.4329 (4)	0.0569 (16)
H2	0.815022	0.464032	0.409826	0.068*
C3	0.9707 (6)	0.6115 (7)	0.4232 (4)	0.0635 (18)
H3	1.047683	0.574782	0.392547	0.076*
C4	0.9953 (6)	0.7307 (7)	0.4591 (4)	0.0668 (18)
H4	1.090460	0.773923	0.453560	0.080*
C5	0.8797 (6)	0.7881 (6)	0.5037 (4)	0.0616 (17)
H5	0.895020	0.869013	0.528319	0.074*
C6	0.7417 (6)	0.7193 (6)	0.5096 (3)	0.0492 (14)
C7	0.6005 (6)	0.7637 (6)	0.5467 (3)	0.0502 (14)
C8	0.4133 (6)	0.8721 (6)	0.6019 (3)	0.0488 (14)
C9	0.3251 (6)	0.9744 (5)	0.6414 (4)	0.0511 (15)
C10	0.3131 (7)	1.1837 (6)	0.6880 (4)	0.0669 (18)
H10	0.359430	1.265472	0.694835	0.080*
C11	0.1694 (7)	1.1648 (6)	0.7181 (4)	0.0646 (18)
H11	0.119229	1.231076	0.745130	0.077*
C12	0.1002 (7)	1.0424 (6)	0.7069 (4)	0.0638 (17)
H12	0.001279	1.026239	0.726126	0.077*
C13	0.1781 (7)	0.9442 (6)	0.6671 (4)	0.0571 (15)
H13	0.133117	0.862298	0.658234	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0312 (5)	0.0473 (6)	0.0557 (7)	−0.0001 (5)	0.0077 (4)	0.0023 (6)

S1	0.0655 (10)	0.0833 (13)	0.0734 (12)	0.0146 (10)	−0.0092 (9)	0.0104 (10)
N1	0.047 (3)	0.060 (3)	0.064 (4)	0.004 (3)	0.010 (3)	0.006 (3)
N2	0.031 (2)	0.060 (3)	0.061 (3)	0.002 (2)	0.008 (2)	0.010 (3)
N3	0.035 (2)	0.057 (3)	0.058 (3)	0.001 (2)	0.008 (2)	0.004 (2)
N4	0.037 (2)	0.047 (3)	0.064 (3)	−0.003 (2)	0.011 (2)	0.000 (2)
N5	0.037 (2)	0.056 (3)	0.057 (3)	−0.007 (2)	0.001 (2)	0.001 (3)
N6	0.054 (3)	0.056 (3)	0.087 (4)	−0.020 (3)	0.005 (3)	−0.004 (3)
N7	0.051 (3)	0.058 (3)	0.070 (4)	−0.006 (3)	0.004 (3)	−0.007 (3)
C1	0.035 (3)	0.065 (4)	0.054 (4)	0.000 (3)	0.010 (3)	−0.003 (3)
C2	0.041 (3)	0.065 (4)	0.066 (4)	0.010 (3)	0.014 (3)	0.014 (3)
C3	0.041 (3)	0.075 (5)	0.076 (5)	0.010 (3)	0.017 (3)	0.014 (4)
C4	0.032 (3)	0.081 (5)	0.088 (5)	−0.006 (3)	0.009 (3)	0.014 (4)
C5	0.042 (3)	0.070 (4)	0.073 (4)	−0.009 (3)	0.008 (3)	0.008 (4)
C6	0.035 (3)	0.054 (4)	0.059 (4)	−0.002 (3)	−0.001 (3)	0.005 (3)
C7	0.041 (3)	0.055 (4)	0.055 (4)	0.001 (3)	0.003 (3)	0.007 (3)
C8	0.041 (3)	0.055 (4)	0.050 (4)	−0.002 (3)	0.002 (3)	0.008 (3)
C9	0.048 (3)	0.043 (4)	0.061 (4)	−0.004 (3)	−0.002 (3)	0.003 (3)
C10	0.067 (4)	0.058 (4)	0.077 (5)	−0.009 (3)	0.012 (4)	−0.017 (4)
C11	0.063 (4)	0.063 (4)	0.068 (5)	0.006 (3)	0.012 (3)	−0.010 (4)
C12	0.060 (4)	0.071 (5)	0.061 (4)	−0.002 (3)	0.011 (3)	0.012 (4)
C13	0.056 (4)	0.051 (4)	0.065 (4)	−0.005 (3)	0.005 (3)	−0.002 (3)

Geometric parameters (Å, º)

Co1—N1	2.113 (5)	N7—C10	1.338 (7)
Co1—N1^{i}	2.113 (5)	C2—H2	0.9300
Co1—N2^{i}	2.164 (4)	C2—C3	1.383 (8)
Co1—N2	2.164 (4)	C3—H3	0.9300
Co1—N3^{i}	2.093 (5)	C3—C4	1.368 (9)
Co1—N3	2.093 (5)	C4—H4	0.9300
S1—C1	1.657 (7)	C4—C5	1.393 (8)
N1—C1	1.154 (7)	C5—H5	0.9300
N2—C2	1.342 (7)	C5—C6	1.375 (7)
N2—C6	1.365 (7)	C6—C7	1.451 (7)
N3—N4	1.372 (6)	C8—C9	1.464 (8)
N3—C7	1.327 (6)	C9—C13	1.377 (7)
N4—C8	1.314 (6)	C10—H10	0.9300
N5—N6	1.427 (6)	C10—C11	1.358 (8)
N5—C7	1.366 (7)	C11—H11	0.9300
N5—C8	1.384 (6)	C11—C12	1.393 (8)
N6—H6A	0.92 (6)	C12—H12	0.9300
N6—H6B	0.86 (6)	C12—C13	1.391 (8)
N7—C9	1.343 (7)	C13—H13	0.9300
N1—Co1—N1^{i}	180.00 (15)	C2—C3—H3	120.2
N1—Co1—N2^{i}	89.83 (17)	C4—C3—C2	119.5 (6)
N1^{i}—Co1—N2^{i}	90.17 (17)	C4—C3—H3	120.2
N1^{i}—Co1—N2	89.82 (17)	C3—C4—H4	119.6

N1—Co1—N2	90.18 (17)	C3—C4—C5	120.8 (6)
N2—Co1—N2^{i}	180.0	C5—C4—H4	119.6
N3—Co1—N1	88.54 (19)	C4—C5—H5	121.6
N3—Co1—N1^{i}	91.46 (19)	C6—C5—C4	116.8 (6)
N3^{i}—Co1—N1^{i}	88.54 (19)	C6—C5—H5	121.6
N3^{i}—Co1—N1	91.46 (19)	N2—C6—C5	122.9 (5)
N3^{i}—Co1—N2	104.51 (17)	N2—C6—C7	110.3 (5)
N3—Co1—N2^{i}	104.51 (17)	C5—C6—C7	126.7 (6)
N3—Co1—N2	75.49 (17)	N3—C7—N5	109.4 (5)
N3^{i}—Co1—N2^{i}	75.49 (17)	N3—C7—C6	120.6 (5)
N3^{i}—Co1—N3	180.0	N5—C7—C6	129.9 (5)
C1—N1—Co1	167.5 (5)	N4—C8—N5	109.7 (5)
C2—N2—Co1	123.6 (4)	N4—C8—C9	124.7 (5)
C2—N2—C6	119.1 (5)	N5—C8—C9	125.6 (5)
C6—N2—Co1	117.2 (3)	N7—C9—C8	117.5 (5)
N4—N3—Co1	136.3 (3)	N7—C9—C13	124.2 (5)
C7—N3—Co1	115.6 (4)	C13—C9—C8	118.3 (5)
C7—N3—N4	108.0 (5)	N7—C10—H10	117.7
C8—N4—N3	107.7 (4)	N7—C10—C11	124.5 (6)
C7—N5—N6	125.9 (4)	C11—C10—H10	117.7
C7—N5—C8	105.1 (4)	C10—C11—H11	121.3
C8—N5—N6	128.9 (5)	C10—C11—C12	117.4 (6)
N5—N6—H6A	106 (4)	C12—C11—H11	121.3
N5—N6—H6B	119 (4)	C11—C12—H12	119.8
H6A—N6—H6B	97 (6)	C13—C12—C11	120.4 (6)
C10—N7—C9	116.8 (5)	C13—C12—H12	119.8
N1—C1—S1	179.3 (6)	C9—C13—C12	116.6 (6)
N2—C2—H2	119.5	C9—C13—H13	121.7
N2—C2—C3	120.9 (6)	C12—C13—H13	121.7
C3—C2—H2	119.5		

Co1—N2—C2—C3	−176.0 (4)	N7—C10—C11—C12	−0.6 (10)
Co1—N2—C6—C5	174.9 (4)	C2—N2—C6—C5	−0.6 (8)
Co1—N2—C6—C7	−9.1 (6)	C2—N2—C6—C7	175.5 (4)
Co1—N3—N4—C8	−179.8 (4)	C2—C3—C4—C5	−1.4 (9)
Co1—N3—C7—N5	−179.6 (3)	C3—C4—C5—C6	0.0 (9)
Co1—N3—C7—C6	2.4 (7)	C4—C5—C6—N2	1.0 (8)
N2—C2—C3—C4	1.8 (9)	C4—C5—C6—C7	−174.4 (5)
N2—C6—C7—N3	4.5 (7)	C5—C6—C7—N3	−179.6 (5)
N2—C6—C7—N5	−173.1 (5)	C5—C6—C7—N5	2.8 (10)
N3—N4—C8—N5	0.8 (6)	C6—N2—C2—C3	−0.8 (8)
N3—N4—C8—C9	−178.4 (5)	C7—N3—N4—C8	−1.6 (6)
N4—N3—C7—N5	1.7 (6)	C7—N5—C8—N4	0.3 (6)
N4—N3—C7—C6	−176.3 (4)	C7—N5—C8—C9	179.5 (5)
N4—C8—C9—N7	−172.5 (5)	C8—N5—C7—N3	−1.2 (6)
N4—C8—C9—C13	6.6 (9)	C8—N5—C7—C6	176.5 (5)
N5—C8—C9—N7	8.4 (8)	C8—C9—C13—C12	177.7 (5)
N5—C8—C9—C13	−172.5 (5)	C9—N7—C10—C11	−1.4 (9)

N6—N5—C7—N3	176.0 (5)	C10—N7—C9—C8	−177.6 (5)
N6—N5—C7—C6	−6.3 (9)	C10—N7—C9—C13	3.4 (9)
N6—N5—C8—N4	−176.8 (5)	C10—C11—C12—C13	0.7 (9)
N6—N5—C8—C9	2.4 (9)	C11—C12—C13—C9	1.0 (9)
N7—C9—C13—C12	−3.2 (9)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···S1^{ii}	0.92 (6)	2.72 (6)	3.481 (7)	140 (5)
N6—H6*B*···N7	0.86 (6)	2.29 (6)	2.847 (7)	122 (5)
C5—H5···N6	0.93	2.51	3.103 (8)	122

Symmetry code: (ii) *x*+1/2, −*y*+3/2, *z*+1/2.

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ^2N^2,N^3]bis(thiocyanato-κN)cobalt(II) (Co_B_300K)

Crystal data

$[Co(NCS)_2(C_{12}H_{10}N_6)_2]$
M_r = 651.61
Monoclinic, $P2_1/n$
a = 11.5855 (6) Å
b = 9.5998 (5) Å
c = 12.8411 (6) Å
β = 101.300 (1)°
V = 1400.48 (12) Å^3
Z = 2
$F(000)$ = 666
D_x = 1.545 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3211 reflections
θ = 2.7–28.2°
μ = 0.81 mm^{-1}
T = 300 K
Prism, orange
0.48 × 0.22 × 0.1 mm

Data collection

Bruker SMART CCD 1K area detector diffractometer
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.805, T_{max} = 0.887
7562 measured reflections
2565 independent reflections
2034 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°, θ_{min} = 2.2°
h = −13→13
k = −11→10
l = −9→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 1.03
2565 reflections
202 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 0.514P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 3 sets of ω scans each set at different φ and/or 2θ angles and each scan (5 s exposure) covering -0.300° degrees in ω. The crystal to detector distance was 4.424 cm.

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	0.5000	0.5000	0.5000	0.03629 (14)
S1	0.47957 (6)	0.70374 (7)	0.14959 (5)	0.04980 (19)
N1	0.51074 (18)	0.5839 (2)	0.35102 (17)	0.0491 (5)
N2	0.54071 (15)	0.7033 (2)	0.57087 (14)	0.0383 (5)
N3	0.33383 (15)	0.5982 (2)	0.48281 (15)	0.0386 (5)
N4	0.22058 (16)	0.5665 (2)	0.43212 (15)	0.0401 (5)
N5	0.22794 (15)	0.7846 (2)	0.48682 (14)	0.0345 (4)
N6	0.19643 (19)	0.9198 (2)	0.5153 (2)	0.0463 (5)
H6A	0.145 (2)	0.906 (3)	0.558 (2)	0.056*
H6B	0.157 (2)	0.957 (3)	0.459 (2)	0.056*
N7	−0.00343 (16)	0.8221 (2)	0.35788 (16)	0.0454 (5)
C1	0.49760 (19)	0.6333 (2)	0.2676 (2)	0.0372 (5)
C2	0.6480 (2)	0.7483 (3)	0.61693 (19)	0.0460 (6)
H2	0.7119	0.6894	0.6181	0.055*
C3	0.6675 (2)	0.8784 (3)	0.6628 (2)	0.0508 (7)
H3	0.7431	0.9061	0.6946	0.061*
C4	0.5742 (2)	0.9659 (3)	0.6607 (2)	0.0497 (7)
H4	0.5856	1.0536	0.6919	0.060*
C5	0.4619 (2)	0.9230 (3)	0.61174 (19)	0.0446 (6)
H5	0.3974	0.9816	0.6084	0.053*
C6	0.44896 (18)	0.7913 (3)	0.56825 (17)	0.0355 (5)
C7	0.33730 (18)	0.7286 (2)	0.51491 (16)	0.0336 (5)
C8	0.15832 (18)	0.6798 (2)	0.43610 (17)	0.0350 (5)
C9	0.03193 (18)	0.6947 (2)	0.39031 (17)	0.0349 (5)
C10	−0.1180 (2)	0.8388 (3)	0.3180 (2)	0.0543 (7)
H10	−0.1440	0.9266	0.2930	0.065*
C11	−0.1991 (2)	0.7346 (3)	0.3116 (2)	0.0571 (8)
H11	−0.2784	0.7519	0.2854	0.069*
C12	−0.1611 (2)	0.6038 (3)	0.3448 (2)	0.0585 (8)
H12	−0.2145	0.5308	0.3414	0.070*
C13	−0.0428 (2)	0.5817 (3)	0.3833 (2)	0.0466 (6)
H13	−0.0143	0.4933	0.4039	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0296 (2)	0.0432 (3)	0.0355 (3)	0.0059 (2)	0.00493 (17)	0.0005 (2)

S1	0.0488 (4)	0.0511 (4)	0.0492 (4)	0.0041 (3)	0.0088 (3)	0.0143 (3)
N1	0.0484 (13)	0.0567 (15)	0.0438 (13)	0.0057 (11)	0.0126 (10)	0.0028 (11)
N2	0.0295 (10)	0.0482 (13)	0.0367 (11)	0.0017 (9)	0.0058 (8)	−0.0008 (9)
N3	0.0315 (10)	0.0432 (12)	0.0396 (11)	0.0019 (9)	0.0034 (8)	−0.0016 (9)
N4	0.0317 (10)	0.0415 (12)	0.0450 (12)	0.0037 (9)	0.0021 (9)	−0.0024 (9)
N5	0.0293 (10)	0.0362 (11)	0.0376 (11)	0.0027 (8)	0.0057 (8)	−0.0012 (9)
N6	0.0384 (12)	0.0407 (13)	0.0583 (15)	0.0055 (10)	0.0061 (10)	−0.0069 (11)
N7	0.0343 (11)	0.0401 (13)	0.0569 (14)	0.0000 (9)	−0.0031 (9)	0.0035 (10)
C1	0.0295 (11)	0.0369 (14)	0.0461 (15)	0.0033 (10)	0.0091 (10)	−0.0024 (11)
C2	0.0300 (12)	0.0605 (18)	0.0462 (15)	0.0019 (12)	0.0042 (10)	−0.0041 (12)
C3	0.0347 (13)	0.069 (2)	0.0469 (16)	−0.0092 (13)	0.0034 (11)	−0.0084 (14)
C4	0.0490 (15)	0.0526 (17)	0.0455 (15)	−0.0072 (13)	0.0045 (12)	−0.0114 (12)
C5	0.0397 (13)	0.0474 (16)	0.0458 (15)	0.0015 (12)	0.0065 (11)	−0.0047 (12)
C6	0.0311 (11)	0.0457 (14)	0.0297 (12)	0.0005 (11)	0.0061 (9)	0.0015 (10)
C7	0.0298 (11)	0.0418 (14)	0.0298 (12)	0.0030 (10)	0.0071 (9)	0.0023 (10)
C8	0.0319 (12)	0.0382 (14)	0.0344 (13)	0.0021 (10)	0.0055 (9)	0.0014 (10)
C9	0.0302 (11)	0.0384 (14)	0.0357 (13)	−0.0011 (10)	0.0056 (9)	−0.0021 (10)
C10	0.0415 (15)	0.0490 (17)	0.0654 (19)	0.0071 (13)	−0.0062 (13)	0.0009 (13)
C11	0.0297 (13)	0.075 (2)	0.0625 (18)	−0.0003 (14)	−0.0007 (12)	−0.0015 (15)
C12	0.0447 (15)	0.069 (2)	0.0579 (18)	−0.0223 (15)	−0.0010 (13)	0.0040 (15)
C13	0.0470 (15)	0.0396 (15)	0.0489 (16)	−0.0048 (12)	−0.0008 (12)	0.0019 (12)

Geometric parameters (Å, º)

Co1—N1^{i}	2.102 (2)	N7—C10	1.336 (3)
Co1—N1	2.102 (2)	C2—H2	0.9300
Co1—N2	2.166 (2)	C2—C3	1.381 (4)
Co1—N2^{i}	2.166 (2)	C3—H3	0.9300
Co1—N3^{i}	2.1161 (18)	C3—C4	1.365 (4)
Co1—N3	2.1161 (18)	C4—H4	0.9300
S1—C1	1.635 (3)	C4—C5	1.392 (3)
N1—C1	1.154 (3)	C5—H5	0.9300
N2—C2	1.339 (3)	C5—C6	1.379 (3)
N2—C6	1.353 (3)	C6—C7	1.469 (3)
N3—N4	1.380 (2)	C8—C9	1.474 (3)
N3—C7	1.316 (3)	C9—C13	1.380 (3)
N4—C8	1.312 (3)	C10—H10	0.9300
N5—N6	1.416 (3)	C10—C11	1.363 (4)
N5—C7	1.359 (3)	C11—H11	0.9300
N5—C8	1.371 (3)	C11—C12	1.371 (4)
N6—H6A	0.89 (3)	C12—H12	0.9300
N6—H6B	0.85 (3)	C12—C13	1.379 (3)
N7—C9	1.330 (3)	C13—H13	0.9300
N1^{i}—Co1—N1	180.0	C2—C3—H3	120.5
N1^{i}—Co1—N2^{i}	89.45 (8)	C4—C3—C2	119.0 (2)
N1^{i}—Co1—N2	90.56 (8)	C4—C3—H3	120.5
N1—Co1—N2^{i}	90.55 (8)	C3—C4—H4	120.2

N1—Co1—N2	89.44 (8)	C3—C4—C5	119.6 (2)
N1^{i}—Co1—N3^{i}	87.09 (8)	C5—C4—H4	120.2
N1^{i}—Co1—N3	92.91 (8)	C4—C5—H5	120.9
N1—Co1—N3	87.09 (8)	C6—C5—C4	118.2 (2)
N1—Co1—N3^{i}	92.91 (8)	C6—C5—H5	120.9
N2^{i}—Co1—N2	180.0	N2—C6—C5	122.7 (2)
N3^{i}—Co1—N2	103.83 (7)	N2—C6—C7	111.8 (2)
N3—Co1—N2	76.17 (7)	C5—C6—C7	125.5 (2)
N3^{i}—Co1—N2^{i}	76.17 (7)	N3—C7—N5	108.88 (19)
N3—Co1—N2^{i}	103.83 (7)	N3—C7—C6	120.4 (2)
N3^{i}—Co1—N3	180.0	N5—C7—C6	130.7 (2)
C1—N1—Co1	169.07 (19)	N4—C8—N5	110.48 (18)
C2—N2—Co1	125.66 (16)	N4—C8—C9	125.1 (2)
C2—N2—C6	117.8 (2)	N5—C8—C9	124.4 (2)
C6—N2—Co1	116.54 (14)	N7—C9—C8	115.8 (2)
N4—N3—Co1	135.45 (15)	N7—C9—C13	123.5 (2)
C7—N3—Co1	114.82 (14)	C13—C9—C8	120.8 (2)
C7—N3—N4	109.00 (18)	N7—C10—H10	118.1
C8—N4—N3	106.15 (19)	N7—C10—C11	123.8 (3)
C7—N5—N6	124.66 (19)	C11—C10—H10	118.1
C7—N5—C8	105.48 (18)	C10—C11—H11	120.7
C8—N5—N6	129.62 (18)	C10—C11—C12	118.6 (2)
N5—N6—H6A	105.2 (18)	C12—C11—H11	120.7
N5—N6—H6B	106.7 (19)	C11—C12—H12	120.4
H6A—N6—H6B	106 (3)	C11—C12—C13	119.2 (2)
C9—N7—C10	116.9 (2)	C13—C12—H12	120.4
N1—C1—S1	179.7 (3)	C9—C13—H13	121.0
N2—C2—H2	118.6	C12—C13—C9	118.0 (2)
N2—C2—C3	122.7 (2)	C12—C13—H13	121.0
C3—C2—H2	118.6		

Co1—N2—C2—C3	−178.53 (19)	N7—C10—C11—C12	−2.2 (4)
Co1—N2—C6—C5	179.02 (18)	C2—N2—C6—C5	−0.7 (3)
Co1—N2—C6—C7	−0.7 (2)	C2—N2—C6—C7	179.64 (19)
Co1—N3—N4—C8	−169.85 (17)	C2—C3—C4—C5	−0.7 (4)
Co1—N3—C7—N5	171.98 (13)	C3—C4—C5—C6	1.1 (4)
Co1—N3—C7—C6	−6.0 (3)	C4—C5—C6—N2	−0.4 (4)
N2—C2—C3—C4	−0.5 (4)	C4—C5—C6—C7	179.2 (2)
N2—C6—C7—N3	4.5 (3)	C5—C6—C7—N3	−175.2 (2)
N2—C6—C7—N5	−173.0 (2)	C5—C6—C7—N5	7.3 (4)
N3—N4—C8—N5	0.7 (2)	C6—N2—C2—C3	1.1 (3)
N3—N4—C8—C9	179.2 (2)	C7—N3—N4—C8	−0.5 (2)
N4—N3—C7—N5	0.2 (2)	C7—N5—C8—N4	−0.5 (2)
N4—N3—C7—C6	−177.79 (18)	C7—N5—C8—C9	−179.1 (2)
N4—C8—C9—N7	−150.0 (2)	C8—N5—C7—N3	0.2 (2)
N4—C8—C9—C13	30.4 (3)	C8—N5—C7—C6	177.9 (2)
N5—C8—C9—N7	28.3 (3)	C8—C9—C13—C12	176.7 (2)
N5—C8—C9—C13	−151.3 (2)	C9—N7—C10—C11	1.8 (4)

N6—N5—C7—N3	175.0 (2)	C10—N7—C9—C8	−178.7 (2)
N6—N5—C7—C6	−7.2 (4)	C10—N7—C9—C13	0.8 (4)
N6—N5—C8—N4	−175.0 (2)	C10—C11—C12—C13	0.0 (4)
N6—N5—C8—C9	6.5 (4)	C11—C12—C13—C9	2.3 (4)
N7—C9—C13—C12	−2.9 (4)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···S1^{ii}	0.89 (3)	2.66 (3)	3.520 (3)	162 (2)
N6—H6*B*···N7	0.85 (3)	2.43 (3)	2.914 (3)	117 (2)
C5—H5···N6	0.93	2.47	3.083 (3)	123

Symmetry code: (ii) *x*−1/2, −*y*+3/2, *z*+1/2.