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

Helen E. Mason, Judith A. K. Howard and Hazel A. Sparkes

The synthesis and structures of bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-$\kappa^2N^2,N^3$]bis(thiocyanato-$\kappa^2N$)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-$\kappa^2N^2,N^3$]bis(thiocyanato-$\kappa^2N$)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/C1/C1/C1 hydrogen bond, C—H/C1/C1/C1 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...
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).

![Scheme 1](image)

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\(_2\)O (1 mmol, 0.281 g) or NiSO\(_4\)\(\cdot\)6H\(_2\)O (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\(_2\)SO\(_4\) 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 (DFM) wherever feasible.

3. Results and discussion

The structure of Co(NCS)\(_2\) (abpt)\(_2\) polymer 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

| Crystal data | 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 |
|--------------|-----------------------------------|-----------------------------------|---------------------------------|-----------------------------------|
| 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\(_6\))\(_2\)] |
| \(M_e\) | 651.61 | 651.61 | 651.39 | 651.39 |
| \(a, b, c (\text{Å})\) | 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) |
| \(c\) (°) | 93.485 (1) | 100.771 (1) | 93.060 (2) | 100.806 (2) |
| \(V (Å^3)\) | 1368.07 (10) | 1371.8 (2) | 0.91 | 0.89 |
| \(μ (\text{mm}^{-1})\) | 0.81 | 0.83 | 0.81 | 0.83 |
| 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 area detector | Bruker SMART CCD 1K area detector |
|---------------|----------------------------------|----------------------------------|---------------------------------|----------------------------------|
| \(T_{\text{min}}, T_{\text{max}}\) | 0.793, 0.919 | 0.755, 0.884 | 0.781, 0.936 | 0.746, 0.948 |
| No. of measured, independent and observed \([I > 2σ(I)]\) reflections | 13341, 2884, 2383 | 13084, 2799, 2363 | 15450, 2819, 2161 | 12077, 2552, 1666 |
| \(R_{\text{int}}\) \((\sin θ/λ)_{\text{max}} (Å^{-1})\) | 0.044 | 0.037 | 0.046 | 0.116 |
| 0.625 | 0.625 | 0.625 | 0.602 |
| \(R[F^2 > 2σ(F^2)], wR(F^2), S\) | 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 |
| Δρ_{max}, Δρ_{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).
asymmetric unit \((Z' = 0.5)\) (Fig. 1). Each of the four complexes consists of an approximately octahedrally coordinated metal centre (Co\(\text{II}\) or Ni\(\text{II}\)) 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\(/\text{C1}/\text{C1}/\text{C1}\) 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\(/\text{C1}/\text{C1}/\text{C1}\) interactions, one between a pyridyl C—H group and 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).

The pair of A polymorphs of the Co\(\text{II}\) or Ni\(\text{II}\) structures are isomorphic 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\(/\text{C1}/\text{C1}/\text{C1}\) hydrogen bonding and C—H\(/\text{C1}/\text{C1}/\text{C1}\) interactions, the structures contain intermolecular \(\pi—\pi\) 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 \(\pi—\pi\) interactions, but in this case each of the pyridyl rings on the abpt ligand is involved in a \(\pi—\pi\) 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 \(\pi—\pi\) 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 \(\sim 9^\circ\), while for B,

![Figure 1](image_url)

**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) \(-x + 1, -y + 1, -z + 1\).]

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

| Structure | Polymorph | \(D—H\cdot\cdot\cdotA\) | \(D—H\) | \(H—A\) | \(D—A\) | \(D—H—A\) |
|-----------|-----------|------------------|---------|---------|---------|------------|
| Co(NCS)\(_2\)(abpt)\(_2\) | A | N6—H6b—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—N4i 0.95 2.67 3.467 (3) 142 | | |
| | B | N6—H6b—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—N4ii 0.95 2.66 3.482 (2) 145 | | |
| Ni(NCS)\(_2\)(abpt)\(_2\) | A | N6—H6b—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—N4i 0.95 2.55 3.437 (3) 141 | | |
| | B | N6—H6b—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—N4ii 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 twist between the rings is $\sim 35^\circ$ (Table 4). This is likely to be the reason for the significantly different $\pi-\pi$ 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
$\pi-\pi$ 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 | 3.63                        | 1.31          |
|                 | B         | N7,C9,C10,C11,C12,C13 | N2,C2,C3,C4,C5,C6 | 3.63                        | 1.31          |
| Ni(NCS)$_2$(abpt)$_2$ | A         | N2,C2,C3,C4,C5,C6 | N7,C9,C10,C11,C12,C13 | 3.63                        | 1.34          |
|                 | B         | N7,C9,C10,C11,C12,C13 | N2,C2,C3,C4,C5,C6 | 3.64                        | 1.34          |

Symmetry codes: (i) $x + 1$, $-y + 2$, $-z + 1$; (ii) $x + \frac{1}{2}$, $-y + \frac{1}{2}$, $z + \frac{1}{2}$; (iii) $x - \frac{1}{2}$, $y - \frac{1}{2}$, $z - \frac{1}{2}$.
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 NiII, 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 \(\sim 9^\circ\) for polymorph A and \(\sim 35^\circ\) 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.

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Computing details

Data collection: SMART (Bruker, 1999) for Co$_A$$_{120}$K, Co$_B$$_{120}$K, Ni$_B$$_{120}$K, Co$_A$$_{300}$K, Co$_B$$_{300}$K; APEX2 (Bruker, 2005) for Ni$_A$$_{120}$K. Cell refinement: SAINT (Bruker, 2003) for Co$_A$$_{120}$K, Co$_B$$_{120}$K, Ni$_B$$_{120}$K, Co$_A$$_{300}$K, Co$_B$$_{300}$K; APEX2 (Bruker, 2005) for Ni$_A$$_{120}$K. Data reduction: SAINT (Bruker, 2003) for Co$_A$$_{120}$K, Co$_B$$_{120}$K, Ni$_B$$_{120}$K, Co$_A$$_{300}$K, Co$_B$$_{300}$K; SAINT-Plus (Bruker, 2013) for Ni$_A$$_{120}$K. For all structures, program(s) used to solve structure: SHELXS (Sheldrick, 2008). Program(s) used to refine structure: SHELXL2018 (Sheldrick, 2015) for Co$_A$$_{120}$K, Co$_B$$_{120}$K, Ni$_A$$_{120}$K, Ni$_B$$_{120}$K, Co$_A$$_{300}$K, Co$_B$$_{300}$K; SHELXL2014 (Sheldrick, 2015) for Co$_B$$_{300}$K. 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$^2$N$_2$,N$_3$]bis(thiocyanato-κN)cobalt(II) (Co$_A$$_{120}$K)

Crystal data

$[\text{Co(NCS)}$_2$(\text{C}_$_{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)$^\circ$

$V = 1404.22$ (17) Å$^3$

$Z = 2$

$F(000) = 666$

$D_r = 1.541$ Mg m$^{-3}$

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

Cell parameters from 6392 reflections

$\theta = 2.4$–$28.4^\circ$

$\mu = 0.81$ mm$^{-1}$

$T = 120$ K

Block, orange

$0.24 \times 0.16 \times 0.11$ mm

Data collection

Bruker SMART CCD 1K area detector diffractometer

Radiation source: sealed X-ray tube

Graphite monochromator

Detector resolution: 7.9 pixels mm$^{-1}$

$\omega$ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2008)

$R_{\text{min}} = 0.793$, $R_{\text{max}} = 0.919$

Refinement

Refinement on $F^2$

$wR(F^2) = 0.093$

Least-squares matrix: full

$S = 1.06$

$R[F^2 > 2\sigma(F^2)] = 0.039$

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  
\[ w = 1/[\sigma(F_o^2) + (0.0335P)^2 + 1.6189P] \]
where \( P = (F_o^2 + 2F_c^2)/3 \)

(\(\Delta/\sigma\))\text{max} < 0.001
\(\Delta\rho_{\text{max}} = 0.58 \text{ e Å}^{-3}\)
\(\Delta\rho_{\text{min}} = -0.27 \text{ e Å}^{-3}\)

**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    | \(U_{\text{iso}}^*/U_{\text{eq}}\) |
|---|------|------|------|---------------------------|
| Co1 | 0.50000 | 0.50000 | 0.50000 | 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) | −0.00003 (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) | 0.0266 (13) | 0.0268 (13) | 0.0021 (10)  | −0.0013 (10) | 0.0035 (10)  |
| C10  | 0.0313 (15) | 0.0322 (14) | 0.0012 (13) | 0.0003 (12)  | −0.0006 (11) | −0.0054 (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, °)

|      |      |      |      |      |      |
|------|------|------|------|------|------|
| Co1—N1 | 2.116 (2) | N7—C10 | 1.342 (3) |
| Co1—N1i | 2.116 (2) | C2—H2 | 0.9500 |
| Co1—N2i | 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—N3i | 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 |
| Bond                  | Angle (°)       | Bond                  | Angle (°)       |
|----------------------|-----------------|----------------------|-----------------|
| N1—Co1—N1i           | 180.00 (11)     | C2—C3—H3             | 120.6           |
| N1—Co1—N2i           | 89.66 (8)       | C4—C3—C2             | 118.9 (3)       |
| N1i—Co1—N2           | 90.34 (8)       | C4—C3—H3             | 120.6           |
| N1i—Co1—N2i          | 89.66 (8)       | C3—C4—H4             | 120.3           |
| N1—Co1—N2            | 90.34 (8)       | C3—C4—C5             | 119.3 (3)       |
| N2—Co1—N2i           | 180.0           | C5—C4—H4             | 120.3           |
| N3i—Co1—N1           | 91.88 (8)       | C4—C5—H5             | 120.7           |
| N3i—Co1—N1i          | 88.12 (8)       | C6—C5—C4             | 118.5 (3)       |
| N3—Co1—N1i           | 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)       |
| N3i—Co1—N2i          | 76.22 (8)       | C5—C6—C7             | 126.7 (2)       |
| N3i—Co1—N2           | 103.78 (8)      | N3—C7—N5             | 108.8 (2)       |
| N3—Co1—N2i           | 103.78 (8)      | N3—C7—C6             | 120.3 (2)       |
| N3—Co1—N3i           | 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           |                      |                 |

**Notes:**

- Co1—N2—C2—C3: $-175.97 (19)$
- Co1—N2—C6—C5: $174.34 (19)$
- Co1—N2—C6—C7: $-7.9 (3)$
- Co1—N3—N4—C8: $179.89 (18)$
- Co1—N3—C7—N5: $-179.68 (15)$
- Co1—N3—C7—N6: $8.03 (3)$
- N2—C2—C3—C4: $1.2 (4)$
- N2—C6—C7—N3: $-173.2 (2)$
- N3—N4—C8—N5: $0.8 (3)$
- N3—N4—C8—C9: $-178.4 (2)$
- N4—N3—C7—N5: $1.2 (3)$
- N4—N3—C7—C6: $-175.9 (2)$
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)
N5—C8—C9—N7  8.8 (4)  C10—C11—C12—C13  1.7 (4)
N5—C8—C9—C13  −171.4 (2)  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, °)

| D—H···A   | D—H  | H···A | D···A | D—H···A |
|-----------|-------|-------|-------|---------|
| N6—H6B···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-κ²N²,N³]bis(thiocyanato-κN)cobalt(II) (Co_B_120K)

Crystal data

[Co(NCS)₂(C₁₂H₁₀N₆)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) Å³

$Z = 2$

F(000) = 666

$D_x = 1.582$ Mg m⁻³

Mo $Kα$ radiation, $λ = 0.71073$ Å

Cell parameters from 7088 reflections

$θ_{max} = 28.3°$

$θ_{min} = 2.7°$

h = −14→14

k = −11→11

l = −15→15

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)

$T_{min} = 0.755$, $T_{max} = 0.884$

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R(F^2 > 2σ(F^2)) = 0.028$

$wR(F^2) = 0.065$

$S = 1.03$

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

$w = 1/[σ^2(F^2) + (0.0223P)^2 + 0.9469P]$

where $P = (F^2 + 2F'^2)/3$

$(Δ/σ)_{max} < 0.001$

Δρ_{max} = 0.26 e Å⁻³

Δρ_{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(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 (6)  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, °)

| Bond          | Distance (Å) | Angle (°) |
|---------------|--------------|-----------|
| Co1—N1        | 2.0987 (15)  | N7—C10    | 1.336 (2) |
| Co1—N1i       | 2.0987 (15)  | C2—H2     | 0.9500    |
| Co1—N2i       | 2.1616 (15)  | C2—C3     | 1.385 (3) |
| Co1—N2        | 2.1616 (15)  | C3—H3     | 0.9500    |
| Co1—N3i       | 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—N1i     | 180.0        | C2—C3—H3  | 120.6     |
N1—Co1—N2      | 89.33 (6)    | C4—C3—C2  | 118.86 (17)|
N1—Co1—N2i     | 90.67 (6)    | C4—C3—H3  | 120.6     |
N1—Co1—N2      | 90.67 (6)    | C3—C4—H4  | 120.3     |
N1—Co1—N2i     | 89.33 (6)    | C3—C4—C5  | 119.49 (18)|
N1—Co1—N3i     | 93.19 (6)    | C5—C4—H4  | 120.3     |

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N1—Co1—N3 86.81 (6)  C4—C5—H5 120.9
N1—Co1—N3 93.19 (6)  C6—C5—C4 118.27 (17)
N1—Co1—N3i 86.81 (6)  C6—C5—H5 120.9
N2—Co1—N2i 180.0  N2—C6—C5 122.73 (16)
N3—Co1—N2i 76.49 (6)  N2—C6—C7 111.63 (15)
N3—Co1—N2 103.50 (6)  N3—C7—N5 108.79 (15)
N3—Co1—N2 76.50 (6)  N3—C7—C6 120.67 (15)
N3—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)  C13—C9—C13 120.8
C8—N4—N3 106.41 (14)  C13—C12—C13 119.03 (18)
C7—N5—N6 124.80 (15)  C10—N7—C13—C12 120.5
C7—N5—C8 105.63 (14)  C10—N7—C13—H13 120.9
C8—N5—N6 129.29 (14)  N7—C10—C11—C12 119.03 (18)
N5—N6—H6A 105.7 (14)  N7—C10—C11—H11 120.8
N5—N6—H6B 105.8 (13)  N7—C10—C11—C12 119.33 (17)
C10—N7—C9 116.60 (16)  C9—C13—C12—C13 120.8
N1—C1—S1 179.51 (17)  N7—C10—C11—H12 120.5
N2—C2—H2 118.6  C9—C13—C12—H12 120.9
N2—C2—C3 122.71 (17)  N7—C10—C11—C12 120.9
C3—C2—C3 118.6
Co1—N2—C2—C3 −178.73 (13)  N7—C10—C11—C12 2.7 (3)
Co1—N2—C6—C5 179.12 (13)  N7—C10—C11—C12 −0.5 (2)
Co1—N2—C6—C7 −1.01 (18)  C2—N2—C6—C5 179.41 (15)
Co1—N3—N4—C8 −168.52 (13)  C2—N2—C6—C7 −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—C4—C5 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)  
N6—N5—C8—C9 6.3 (3)  
N7—C9—C13—C12 −3.3 (3)  
Symmetry code: (i) −x+1, −y+1, −z+1.

Hydrogen-bond geometry (Å, °)

| D—H···A  | D—H  | H···A  | D···A  | D—H···A  |
|----------|------|-------|-------|----------|
| N6—H6A···S1ii  | 0.89 (2) | 2.63 (2) | 3.4758 (17) | 159.9 (18) |
| N6—H6B···N7  | 0.90 (2) | 2.41 (2) | 2.914 (2) | 115.6 (18) |
| 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-κ²N₂,N₃]bis(thiocyanato-κN)nickel(II) (Ni_A_120K)

Crystal data

[Ni(NCS)₂(C₁₂H₁₀N₆)₂]  
F(000) = 668  
Mᵣ = 651.39  
Monoclinic, P₂₁/n  
a = 8.4041 (7) Å  
b = 10.0681 (9) Å  
c = 16.2360 (14) Å  
β = 93.060 (2)°  
V = 1371.8 (2) Å³  
Z = 2  
Dₐ = 1.577 Mg m⁻³  
Mo Kα 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  
F(000) = 668  
Dₐ = 1.577 Mg m⁻³  
Mo Kα 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)  
Tmin = 0.781, Tmax = 0.936  
h = −10→10  
k = −12→12  
l = −20→20  
15450 measured reflections  
2819 independent reflections  
2161 reflections with I > 2σ(I)  
Rint = 0.046  
θmax = 26.4°, θmin = 2.4°  
Rmax = 2.4°  
h = −10→10  
k = −12→12  
l = −20→20

Refinement

Refinement on F²  
Least-squares matrix: full  
R[F² > 2σ(F²)] = 0.037  
wR(F²) = 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  
Hydrogen atom parameters constrained  
where P = (F² + 2Fc²)/3  
(w = 1/[(σ²(Fc²) + (0.037P)² + 0.9816P)]  
(Δσ/σ)max < 0.001  
Δρmax = 0.48 e Å⁻³  
Δρmin = −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)

| Atom | x   | y   | z   | Uiso*/Ueq |
|------|-----|-----|-----|-----------|
| Ni1  | 0.50 | 0.50 | 0.50 | 0.0186 (13) |
| S1   | 0.26 | 0.72 | 0.26 | 0.0308 (18) |
| N1   | 0.39 | 0.57 | 0.39 | 0.0232 (5)  |
| N2   | 0.72 | 0.59 | 0.47 | 0.0215 (5)  |
| N3   | 0.47 | 0.69 | 0.54 | 0.0227 (5)  |
| N4   | 0.35 | 0.76 | 0.59 | 0.0206 (5)  |
| N5   | 0.57 | 0.89 | 0.58 | 0.0221 (5)  |
| N6   | 0.68 | 0.98 | 0.59 | 0.0283 (5)  |
| H6A  | 0.74 | 0.96 | 0.65 | 0.034*      |
| H6B  | 0.63 | 1.06 | 0.61 | 0.0266 (6)  |
| N7   | 0.97 | 1.09 | 0.42 | 0.0213 (5)  |
| C1   | 1.01 | 0.52 | 0.43 | 0.0238 (6)  |
| C2   | 1.01 | 0.61 | 0.45 | 0.0281 (6)  |
| H2   | 0.81 | 0.45 | 0.40 | 0.029*      |
| C3   | 0.97 | 0.60 | 0.41 | 0.0266 (6)  |
| H3   | 1.05 | 0.56 | 0.39 | 0.032*      |
| C4   | 1.00 | 0.72 | 0.45 | 0.0281 (6)  |
| H4   | 1.10 | 0.77 | 0.45 | 0.034*      |
| C5   | 0.89 | 0.78 | 0.50 | 0.0252 (6)  |
| H5   | 0.90 | 0.86 | 0.53 | 0.030*      |
| C6   | 0.74 | 0.71 | 0.51 | 0.0221 (5)  |
| C7   | 0.60 | 0.77 | 0.65 | 0.0216 (5)  |
| C8   | 0.42 | 0.87 | 0.60 | 0.0223 (5)  |
| C9   | 0.32 | 0.98 | 0.67 | 0.0223 (6)  |
| C10  | 0.31 | 1.19 | 0.69 | 0.0246 (6)  |
| H10  | 0.36 | 1.28 | 0.69 | 0.032*      |
| C12  | 0.16 | 1.18 | 0.72 | 0.0256 (6)  |
| H12  | 0.12 | 1.24 | 0.75 | 0.031*      |
| C11  | 0.09 | 1.05 | 0.71 | 0.0266 (6)  |
| H11  | −0.01 | 1.03 | 0.73 | 0.032*      |
| C13  | 0.17 | 0.95 | 0.67 | 0.0247 (6)  |
| H10  | 0.13 | 0.86 | 0.66 | 0.030*      |

Atomic displacement parameters (Å²)

| Atom | U¹¹ | U²² | U³³ | U¹² | U¹³ | U²³ |
|------|-----|-----|-----|-----|-----|-----|
| 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) |
Geometric parameters (Å, °)

| Bond                  | Distance (Å) | Angle (°)   |
|-----------------------|--------------|-------------|
| Ni1—N1i               | 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—N2i               | 2.1076 (19)  | C3—H3       | 0.9500    |
| Ni1—N3                | 2.043 (2)    | C3—C4       | 1.373 (4) |
| Ni1—N3i               | 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    |

N1i—Ni1—N1          180.0  C2—C3—H3   120.4
N1—Ni1—N2i         89.60 (8)  C4—C3—C2  119.1 (2)
N1i—Ni1—N2         89.60 (8)  C4—C3—H3   120.4
N1—Ni1—N2          90.40 (8)  C3—C4—H4   120.3
N1i—Ni1—N2i        90.40 (8)  C3—C4—C5  119.4 (2)
N2i—Ni1—N2         180.0  C5—C4—H4   120.3
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| N3—Ni1—N1           | 88.21 (8)    | C4—C5—H5            | 120.8        |
| N3—Ni1—Ni1i         | 91.79 (8)    | C6—C5—C4            | 118.4 (2)    |
| N3i—Ni1—N1i         | 88.21 (8)    | C6—C5—H5            | 120.8        |
| N3i—Ni1—N1          | 91.79 (8)    | N2—C6—C5            | 122.4 (2)    |
| N3i—Ni1—N2i         | 102.19 (8)   | N2—C6—C7            | 110.9 (2)    |
| N3i—Ni1—N2i         | 77.81 (8)    | C5—C6—C7            | 126.6 (2)    |
| N3i—Ni1—N2          | 77.81 (8)    | N3—C7—N5            | 108.7 (2)    |
| N3i—Ni1—N3i         | 102.19 (8)   | N3—C7—C6            | 119.9 (2)    |
| N3—Ni1—N3i          | 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            | 105.5 (2)    | C13—C12—H12         | 120.7        |
| N5—N6—H6A           | 129.4 (2)    | C11—C12—C13         | 118.6 (2)    |
| N5—N6—H6B           | 101.7 (17)   | C11—C12—H12         | 120.7        |
| H6A—N6—H6B          | 106.7 (19)   | C12—C11—H11         | 120.5        |
| C13—N7—C9           | 116.9 (2)    | C12—C11—C10         | 119.1 (2)    |
| N1—C1—S1            | 179.4 (2)    | C10—C11—H11         | 120.5        |
| N2—C2—H2            | 118.9        | C9—C10—H10          | 121.0        |
| N2—C2—C3            | 122.3 (2)    | C11—C10—C9          | 117.9 (2)    |
| C3—C2—H2            | 118.9        | C11—C10—H10         | 121.0        |
| 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, °)

| D—H···A | D—H  | H···A  | D···A  | D—H···A |
|---------|------|-------|-------|---------|
| N6—H6A···S1ii | 0.98 (3) | 2.54 (3) | 3.404 (3) | 146 (2) |
| N6—H6B···N7 | 0.88 (3) | 2.14 (3) | 2.848 (3) | 137 (3) |
| C2—H2···N4i | 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-κ²N₂,N₃]bis(thiocyanato-κN)nickel(II) (Ni_B_120K)

Crystal data

[Ni(NCS)₂(C₁₂H₁₀N₆)₂]  
F(000) = 668  
M_r = 651.39  
Monoclinic, P2₁/n  
a = 11.5860 (14) Å  
b = 9.5489 (12) Å  
c = 12.8132 (16) Å  
β = 100.806 (2)°  
V = 1392.4 (3) Å³  
Z = 2  

Data collection

Bruker SMART CCD 1K area detector  
Diffractionometer  
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  

Refinement

Refinement on F²  
Least-squares matrix: full  
R[F² > 2σ(F²)] = 0.058  
wR(F²) = 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  
where P = (F² + 2F_C²)/3  
(Δ/σ)max < 0.001  
Δρ_max = 0.61 e Å⁻³  
Δρ_min = −0.66 e Å⁻³  

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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     | Ueq  |
|----|-------|-------|-------|------|
| 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) |
| 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)  |
supporting information

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

\[Geometric\ parameters\ (\text{Å}, {^\circ})\]

\[
\begin{array}{cccc}
\text{Ni1—N1} & 2.080 (5) & \text{N7—C13} & 1.331 (6) \\
\text{Ni1—N1i} & 2.080 (5) & \text{C2—H2} & 0.9500 \\
\text{Ni1—N2} & 2.126 (4) & \text{C2—C3} & 1.388 (7) \\
\text{Ni1—N2} & 2.126 (4) & \text{C3—H3} & 0.9500 \\
\text{Ni1—N3} & 2.098 (4) & \text{C3—C4} & 1.390 (7) \\
\text{Ni1—N3i} & 2.098 (4) & \text{C4—H4} & 0.9500 \\
\text{S1—C1} & 1.651 (5) & \text{C4—C5} & 1.395 (7) \\
\text{N1—C1} & 1.184 (6) & \text{C5—H5} & 0.9500 \\
\text{N2—C2} & 1.359 (6) & \text{C5—C6} & 1.376 (7) \\
\text{N2—C6} & 1.375 (6) & \text{C6—C7} & 1.487 (7) \\
\text{N3—N4} & 1.391 (5) & \text{C8—C9} & 1.482 (7) \\
\text{N3—C7} & 1.321 (6) & \text{C9—C10} & 1.386 (7) \\
\text{N4—C8} & 1.325 (6) & \text{C13—H13} & 0.9500 \\
\text{N5—N6} & 1.429 (6) & \text{C13—C12} & 1.383 (7) \\
\text{N5—C7} & 1.371 (6) & \text{C12—H12} & 0.9500 \\
\text{N5—C8} & 1.389 (6) & \text{C12—C11} & 1.393 (8) \\
\text{N6—H6A} & 0.84 (5) & \text{C11—H11} & 0.9500 \\
\text{N6—H6B} & 0.84 (6) & \text{C11—C10} & 1.392 (7) \\
\text{N7—C9} & 1.376 (6) & \text{C10—H10} & 0.9500 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{N1—Ni1—N1i} & 180.0 & \text{C2—C3—H3} & 120.8 \\
\text{N1—Ni1—N2} & 89.98 (17) & \text{C2—C3—C4} & 118.3 (5) \\
\text{N1—Ni1—N2} & 90.02 (17) & \text{C4—C3—H3} & 120.8 \\
\text{N1—Ni1—N2i} & 90.02 (17) & \text{C3—C4—H4} & 120.0 \\
\text{N1—Ni1—N2i} & 89.98 (17) & \text{C3—C4—C5} & 120.0 (5) \\
\text{N1—Ni1—N3} & 86.93 (16) & \text{C5—C4—H4} & 120.0 \\
\end{array}
\]
| Bond/Rotation | Value (°) | Value (°) | Value (°) |
|--------------|----------|----------|----------|
| 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 i—Ni1—N2 | 101.90 (16) | C5—C6—C7 | 125.9 (5) |
| N3 i—Ni1—N2 i | 101.90 (16) | N3—C7—N5 | 108.5 (4) |
| N3—Ni1—N3 i | 86.93 (16) | N3—C7—C6 | 121.1 (4) |
| N4—N3—Ni1 | 136.0 (3) | N5—C7—C6 | 130.4 (5) |
| C7—N3—Ni1 | 113.5 (3) | N4—C8—N5 | 110.2 (4) |
| C7—N3—N4 | 109.7 (4) | N4—C8—C9 | 125.3 (5) |
| C8—N4—N3 | 105.9 (4) | N5—C8—C9 | 124.5 (4) |
| C7—N5—N6 | 124.3 (4) | C5—C6—C7 | 115.3 (4) |
| C7—N5—C8 | 105.7 (4) | C12—C13—H13 | 120.7 |
| C8—N5—N6 | 129.7 (4) | C12—C13—H13 | 117.8 |
| C8—N6—H6A | 108 (4) | C13—C12—C11 | 118.6 (5) |
| N5—N6—H6B | 102 (4) | C13—C12—C11 | 120.7 |
| 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 | | |

| Bond/Rotation | Value (°) |
|--------------|----------|
| Ni1—N2—C2—C3 | −178.1 (4) |
| Ni1—N2—C6—C5 | 178.8 (4) |
| Ni1—N2—C6—C7 | −0.7 (5) |
| Ni1—N3—N4—C8 | −169.4 (4) |
| Ni1—N3—C7—N5 | 172.2 (3) |
| Ni1—N3—C7—C6 | −6.0 (6) |
| N2—C2—C3—C4 | −1.4 (8) |
| N2—C6—C7—N3 | 4.5 (7) |
| N2—C6—C7—N5 | −173.3 (5) |
| N3—N4—C8—N5 | 0.0 (6) |
| N3—N4—C8—C9 | −179.7 (5) |
| N4—N3—C7—N5 | 0.5 (6) |
| N4—N3—C7—C6 | −177.7 (4) |
| N4—C8—C9—N7 | −150.3 (5) |
| N4—C8—C9—C10 | 30.6 (8) |
| N5—C8—C9—N7 | 30.0 (7) |
| N5—C8—C9—C10 | −149.1 (5) |
| N6—N5—C7—N3 | 174.7 (4) |
| N6—N5—C7—C6 | −7.4 (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, °)

| D—H···A     | D—H  | H···A  | D···A  | D—H···A |
|-------------|--------|--------|--------|--------|
| N6—H6A···S1ii | 0.84 (5) | 2.70 (5) | 3.496 (5) | 159 (5) |
| N6—H6B···N7  | 0.84 (6) | 2.52 (5) | 2.950 (6) | 112 (4) |
| C2—H2···N4i  | 0.95   | 2.59   | 3.403 (7) | 144    |
| C5—H5···N6   | 0.95   | 2.48   | 3.104 (7) | 123    |
| C10—H10···S1iii | 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-$\kappa^2N_2,N_3$]bis(thiocyanato-$\kappa^N$)cobalt(II) (Co_A_300K)

Crystal data
[Co(NCS)$_2$(C$_{12}$H$_{10}$N$_6$)$_2$]  
$F(000) = 666$

$M_r = 651.61$

Monoclinic, $P2_1/n$

Cell parameters from 1789 reflections

$a = 8.487$ (5) Å

$D_x = 1.507$ Mg m$^{-3}$

Radiation source: sealed X-ray tube

$\lambda = 0.71073$ Å

Cell parameters from 1789 reflections

$\theta = 2.3$–23.5°

$\mu = 0.79$ mm$^{-1}$

$\beta = 93.419$ (13)°

$T = 300$ K

$V = 1435.9$ (14) Å$^3$

$Z = 2$

$\Delta \rho_{\text{max}} = 0.36$ e Å$^{-3}$

Data collection

Bruker SMART CCD 1K area detector diffractometer

7130 measured reflections

2605 independent reflections

1378 reflections with $I > 2\sigma(I)$

$\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$\omega$ scans

$R_{\text{int}} = 0.087$

Absorption correction: multi-scan

(SADABS; Bruker, 2008)

$T_{\text{min}} = 0.683, T_{\text{max}} = 0.921$

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

$w = 1/[\sigma^2(F^2) + (0.0716P)^2 + 0.6349P]$

where $P = (F^2 + 2F^2)/3$

$(\Delta F)_{\text{max}} < 0.001$

$\Delta F_{\text{max}} = 0.36$ e Å$^{-3}$

$\Delta F_{\text{min}} = -0.47$ e Å$^{-3}$

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Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 3 sets of $\omega$ scans each set at different $\phi$ and/or $2\theta$ angles and each scan (12 s exposure) covering -0.300° degrees in $\omega$. 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 ($\AA^2$)

|     | x     | y     | z     | $U_{eq}$/$U_{eq}$ |
|-----|-------|-------|-------|-------------------|
| 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 ($\AA^2$)

|     | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|-----|----------|----------|----------|----------|----------|----------|
| Co1 | 0.0312 (5) | 0.0473 (6) | 0.0557 (7) | -0.0001 (5) | 0.0077 (4) | 0.0023 (6) |
Geometric parameters (Å, °)

|        |         |         |         |         |         |         |
|--------|---------|---------|---------|---------|---------|---------|
| Co1—N1 | 2.113 (5) | N7—C10 | 1.338 (7) |
| Co1—N1i | 2.113 (5) | C2—H2 | 0.9300 |
| Co1—N2i | 2.164 (4) | C2—C3 | 1.383 (8) |
| Co1—N2 | 2.164 (4) | C3—H3 | 0.9300 |
| Co1—N3i | 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—N1i 180.00 (15)  C2—C3—H3 120.2
N1—Co1—N2i 89.83 (17)  C4—C3—C2 119.5 (6)
N1—Co1—N2 90.17 (17)  C4—C3—H3 120.2
N1—Co1—N2 89.82 (17)  C3—C4—H4 119.6
| Bond   | Distance (Å) | Bond   | Distance (Å) | Bond   | Distance (Å) |
|--------|--------------|--------|--------------|--------|--------------|
| N1—Co1—N2 | 90.18 (17)  | C3—C4—C5 | 120.8 (6)    |        |
| N2—Co1—N2i | 180.0       | C5—C4—H4 | 119.6        |        |
| N3—Co1—N1 | 88.54 (19)  | C4—C5—H5 | 121.6        |        |
| N3—Co1—N1i | 91.46 (19)  | C6—C5—C4 | 116.8 (6)    |        |
| N3—Co1—N1 | 88.54 (19)  | C6—C5—H5 | 121.6        |        |
| N3—Co1—N2 | 104.51 (17) | N2—C6—C7 | 110.3 (5)    |        |
| N3—Co1—N2i | 104.51 (17) | N2—C6—C7 | 126.7 (6)    |        |
| N3—Co1—N2 | 75.49 (17)  | N3—C7—N5 | 109.4 (5)    |        |
| N3—Co1—N2i | 75.49 (17)  | N3—C7—N5 | 120.6 (5)    |        |
| N3—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)   | C13—C9—C8 | 118.3 (5)   |        |
| C8—N4—N3 | 107.7 (4)   | N7—C10—H10 | 117.7   |        |
| C7—N5—N6 | 125.9 (4)   | N7—C10—C11 | 124.5 (6) |        |
| C7—N5—C8 | 105.1 (4)   | C11—C10—H10 | 117.7  |        |
| C8—N5—N6 | 128.9 (5)   | C10—C11—H11 | 121.3   |        |
| N5—N6—H6A | 106 (4)     | C10—C11—C12 | 117.4 (6) |        |
| N5—N6—H6B | 119 (4)     | C12—C11—H11 | 121.3  |        |
| H6A—N6—H6B | 97 (6)      | C11—C12—H12 | 119.8  |        |
| C10—N7—C9 | 116.8 (5)   | C13—C12—C11 | 120.4 (6) |        |
| N1—C1—S1 | 179.3 (6)   | C13—C12—H12 | 119.8  |        |
| N2—C2—H2 | 119.5       | C9—C13—C12 | 116.6 (6) |        |
| N2—C2—C3 | 120.9 (6)   | C9—C13—H13 | 121.7   |        |
| C3—C2—H2 | 119.5       | C12—C13—H13 | 121.7  |        |
| 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) |        |
**Hydrogen-bond geometry (Å, †)**

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N6—H6A···S1ii | 0.92 (6) | 2.72 (6) | 3.481 (7) | 140 (5) |
| N6—H6B···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.

**Crystal data**

Bis[4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole-κ²N₂,N³]bis(thiocyanato-κN)cobalt(II) (Co_B_300K)

F(000) = 666

\[ M_r = 651.61 \]

Monoclinic, \( P2_1/n \)

\[ a = 11.5855 (6) \, \text{Å} \]

\[ b = 9.5998 (5) \, \text{Å} \]

\[ c = 12.8411 (6) \, \text{Å} \]

\[ \beta = 101.300 (1) ^\circ \]

\[ V = 1400.48 (12) \, \text{Å}^3 \]

\[ Z = 2 \]

\( \mu = 0.81 \, \text{mm}^{-1} \)

\( T = 300 \, \text{K} \)

Prism, orange

0.48 \times 0.22 \times 0.1 \, \text{mm}

**Data collection**

Bruker SMART CCD 1K area detector

Graphite monochromator

Detector resolution: 7.9 pixels mm\(^{-1}\)

\( \omega \) scans

Absorption correction: multi-scan

(SADABS; Bruker, 2008)

\( T_{\text{min}} = 0.805, T_{\text{max}} = 0.887 \)

\( I = -9 \rightarrow 15 \)

**Refinement**

Refinement on \( F^2 \)

Least-squares matrix: full

\( R(F^2) = 0.034 \)

\( wR(F^2) = 0.079 \)

\( S = 1.03 \)

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

\( w = 1/\sigma^2(F_c^2) + (0.0314P)^2 + 0.514P \)

\( P = (F_c^2 + 2F_s^2)/3 \)

\( \Delta r_{\text{max}} = 0.22 \, \text{e} \, \text{Å}^{-3} \)

\( \Delta r_{\text{min}} = -0.27 \, \text{e} \, \text{Å}^{-3} \)
**Special details**

**Experimental.** The data collection nominally covered a full sphere of reciprocal space by a combination of 3 sets of $\omega$ scans each set at different $\varphi$ and/or $2\theta$ angles and each scan (5 s exposure) covering -0.300° degrees in $\omega$. 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    | Uiso */ Ueq |
|-----|------|------|------|-------------|
| Co1 | 0.500 | 0.500 | 0.500 | 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)**

|     | U₁₁ | U₂₂ | U₃₃ | U₁₂ | U₁₃ | U₂₃ |
|-----|-----|-----|-----|-----|-----|-----|
| Co1 | 0.0296 (2) | 0.0432 (3) | 0.0355 (3) | 0.0059 (2) | 0.00493 (17) | 0.0005 (2) |

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### Geometric parameters (Å, °)

| Bond / Angle | Distance / Angle |
|--------------|------------------|
| Co1—N1i     | 2.102 (2)        |
| Co1—N1      | 2.102 (2)        |
| Co1—N2      | 2.166 (2)        |
| Co1—N2i     | 2.166 (2)        |
| Co1—N3i     | 2.1161 (18)      |
| Co1—N3      | 2.1161 (18)      |
| S1—C1       | 1.635 (3)        |
| N1—C1       | 1.154 (3)        |
| N2—C2       | 1.339 (3)        |
| N2—C6       | 1.355 (3)        |
| N3—N4       | 1.380 (2)        |
| N3—C7       | 1.316 (3)        |
| N4—C8       | 1.312 (3)        |
| N5—N6       | 1.416 (3)        |
| N5—C7       | 1.359 (3)        |
| N5—C8       | 1.371 (3)        |
| N6—H6A      | 0.89 (3)         |
| N6—H6B      | 0.85 (3)         |
| N7—C9       | 1.330 (3)        |
| N1—Co1—N1   | 180.0            |
| N1—Co1—N2   | 89.45 (8)        |
| N1—Co1—N2i  | 90.56 (8)        |
| N1—Co1—N2i  | 90.55 (8)        |
| Bond/Rotation | Distance (Å) | Angle (°) | Temperature Factor (Å²) |
|--------------|-------------|-----------|------------------------|
| N1—Co1—N2   | 89.44 (8)   | C3—C4—C5 | 119.6 (2)              |
| N1—Co1—N3   | 92.91 (8)   | C4—C5—C6 | 120.2                  |
| N1—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'  | 87.09 (8)   | C6—C5—H5 | 120.9                  |
| N2—Co1—N2   | 180.0       | C5—C6—C7 | 122.7 (2)              |
| N3—Co1—N2   | 103.83 (7)  | N2—C6—C7 | 111.8 (2)              |
| N3—Co1—N2'  | 103.83 (7)  | N2—C6—C7 | 111.8 (2)              |
| N3—Co1—N3   | 180.0       | C5—C6—C7 | 125.5 (2)              |
| N3—Co1—N3'  | 180.0       | N3—C7—N5 | 108.88 (19)            |
| N4—Co1—N3   | 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) | C7—C10—H10 | 118.1                 |
| C8—N4—N3    | 106.27 (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—C13 | 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)    | C5—C6—C7—N3 | −175.2 (2)      |
| N2—C6—C7—N3 | 4.5 (3)     | C5—C6—C7—N5 | 7.3 (4)          |
| N2—C6—C7—N5 | −173.0 (2)  | C6—N2—C2—C3 | 1.1 (3)          |
| N3—N4—C8—N5 | 0.7 (2)     | C7—N3—N4—C8 | −0.5 (2)         |
| N3—N4—C8—C9 | 179.2 (2)   | C7—N5—C8—N4 | −0.5 (2)         |
| N4—N3—C7—N5 | 0.2 (2)     | C7—N5—C8—C9 | −179.1 (2)      |
| N4—N3—C7—C6 | −177.79 (18) | C8—N5—C7—N3 | 0.2 (2)         |
| N4—C8—C9—N7 | −150.0 (2)  | C8—N5—C7—C6 | 177.9 (2)       |
| N4—C8—C9—C13 | 30.4 (3)    | C8—C9—C13—C12 | 176.7 (2)     |
| N5—C8—C9—N7 | 28.3 (3)    | C9—N7—C10—C11 | 1.8 (4)        |
| N5—C8—C9—C13 | −151.3 (2)  |               |                       |
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, °)

\[
\begin{array}{cccccc}
D—H···A & D—H & H···A & D···A & D—H···A \\
N6—H6A···S1ii & 0.89 (3) & 2.66 (3) & 3.520 (3) & 162 (2) \\
N6—H6B···N7 & 0.85 (3) & 2.43 (3) & 2.914 (3) & 117 (2) \\
C5—H5···N6 & 0.93 & 2.47 & 3.083 (3) & 123 \\
\end{array}
\]

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