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Bis(4-aminopyridinium) tetrathiocyanatocobaltate(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.063
wR factor = 0.149
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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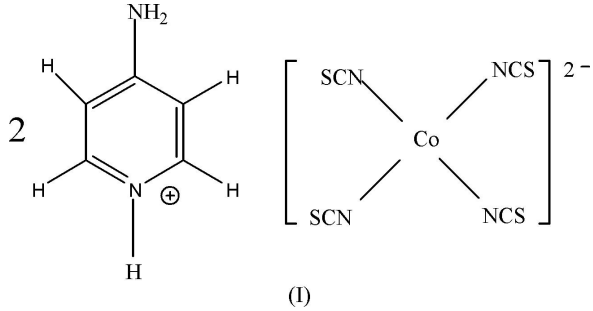
The title structure, $(C_5H_7N_2)_2[Co(NCS)_4]$, comprises discrete monovalent 4-aminopyridinium cations and divalent tetrathiocyanatocobaltate(II) anions. The cations and anions are linked *via* N—H···S hydrogen bonds [N···S = 3.264 (4)–3.640 (6) Å] to form a three-dimensional framework.

Comment

The Co atom of the anion in the title salt, (I), is coordinated by four N atoms from four thiocyanate groups in a slightly distorted tetrahedral geometry (see Table 1). In the crystal structure, there are hydrogen bonds between NH groups and S atoms, in which the NH donor groups are from both amino groups and pyridine ring N atoms (see Table 2) and the resulting N—H···S hydrogen bonds form a three-dimensional framework (see Fig. 2). In addition, there are significant π–π stacking interactions between neighbouring pyridine rings; the relevant distances are $Cg1\cdots Cg1^{i}$ = 3.548 (3) Å and $Cg1\cdots 1^{i}_{perp}$ = 3.306 Å, and $Cg2\cdots Cg2^{ii}$ = 3.925 (4) Å and $Cg2\cdots 2^{ii}_{perp}$ = 3.368 Å [symmetry codes: (i) $1-x, 1-y, -z$; (ii) $-x, 1-y, -z$; $Cg1$ and $Cg2$ are the centroids of the N6/C5–C9 and N7/C10–C14 rings, respectively; $CgI\cdots J_{perp}$ is the perpendicular distance from CgI to ring J].



(I)

Experimental

4-Aminopyridine (0.0574 g, 0.610 mmol) was added to an aqueous solution (15 ml) containing $Co(ClO_4)_2\cdot 6H_2O$ (0.1102 g, 0.301 mmol) and sodium thiocyanate (0.0511 g, 0.630 mmol), and the solution was stirred for a few minutes. Blue single crystals were obtained after the solution was allowed to stand at room temperature for four weeks.

Crystal data

$(C_5H_7N_2)_2[Co(NCS)_4]$
M_r = 481.50
Monoclinic, $P2_1/c$
a = 14.118 (2) Å
b = 9.1179 (14) Å
c = 16.756 (3) Å
β = 98.839 (2)°
V = 2131.4 (6) Å^3
Z = 4
D_x = 1.501 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2201 reflections
θ = 2.6–22.4°
μ = 1.21 mm^{-1}
T = 298 (2) K
Prism, blue
0.25 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.751, T_{max} = 0.909
11075 measured reflections
3936 independent reflections
2795 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.5°
$h = -17 \rightarrow 17$
$k = -11 \rightarrow 10$
$l = -20 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.149
S = 1.05
3936 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 1.614P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	1.939 (4)	Co1—N3	1.951 (4)
Co1—N4	1.944 (4)	Co1—N2	1.956 (4)
N1—Co1—N4	109.84 (16)	N1—Co1—N2	107.78 (17)
N1—Co1—N3	115.66 (18)	N4—Co1—N2	114.37 (16)
N4—Co1—N3	101.76 (17)	N3—Co1—N2	107.56 (16)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N6—H7···S1^{i}	0.86	2.54	3.264 (4)	142
N5—H4B···S4^{ii}	0.86	2.75	3.540 (5)	154
N7—H13A···S2^{iii}	0.86	2.53	3.359 (7)	163
N8—H9A···S3^{iv}	0.86	2.71	3.567 (6)	176
N8—H10B···S2^{v}	0.86	2.79	3.640 (6)	170

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

All H atoms were placed in calculated positions and included in the final cycles of refinement using a riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2$_{eq}$(C); N—H = 0.86 Å and U_{iso}(H) = 1.2$_{eq}$(N)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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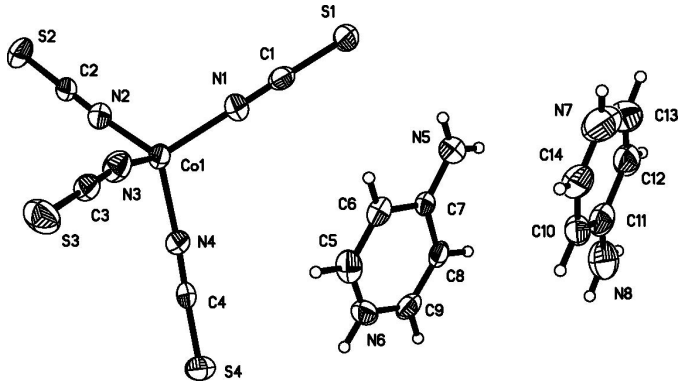

Figure 1
View of the title compound, showing the atom-numbering scheme. Ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

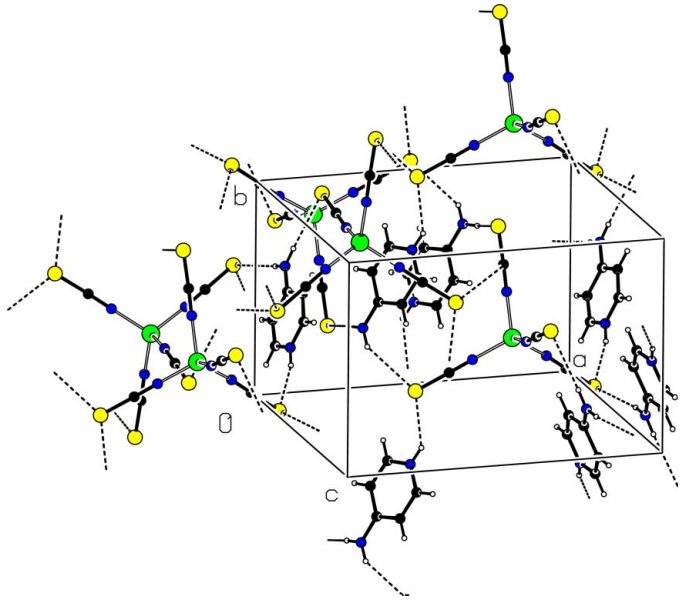

Figure 2
Packing diagram (Spek, 2003), showing N—H···S hydrogen bonds as dashed lines. Colour codes: green Co, yellow S, blue N and black C.

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