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Key indicators

Single-crystal X-ray study
 $T = 120$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.028
 wR factor = 0.119
 Data-to-parameter ratio = 20.7

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

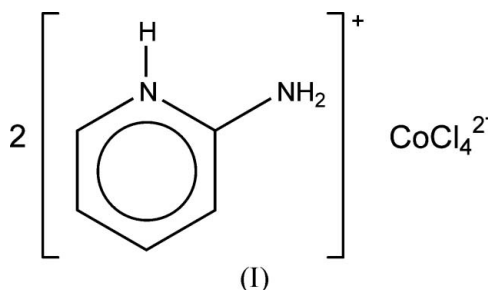
Bis(2-aminopyridinium) tetrachlorocobalt(II)

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In the crystal structure of the title compound, $(\text{C}_5\text{H}_7\text{N}_2)_2\text{[CoCl}_4\text{]}$, the Co^{II} ion is coordinated by four chloride ions. The Co atom lies on a crystallographic twofold rotation axis. The structure is stabilized by an extensive network of $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Comment

2-Aminopyridine is used in the manufacture of pharmaceuticals, especially antihistaminic drugs (Windholz, 1976). As part of our investigation of the reactions of 2-aminopyridine with metals, we report here the crystal structure of the title compound, (I).



The asymmetric unit of (I) contains a 2-aminopyridinium cation and half of a $[\text{CoCl}_4]^{2-}$ anion. The Co atom lies on a crystallographic twofold rotation axis. Protonation of atom N1 of the 2-aminopyridine results in the widening of the $\text{C}2-\text{N}1-\text{C}6$ angle to 122.7 (2)°. This compares with 117.7 (1)° in neutral 2-aminopyridine (Chao *et al.*, 1975). The bond lengths and angles in (I) are comparable to those in other 2-aminopyridinium complexes (Bis & Zaworotko, 2005; Smith *et al.*, 2000; Jebas & Balasubramanian, 2006). The pyridinium ring deviates somewhat from planarity, with a maximum deviation from the mean plane of 0.026 (2) Å for atom C6.

The anion exhibits tetrahedral geometry, with the Co^{II} ion surrounded by four Cl atoms, with $\text{Cl}-\text{Co}-\text{Cl}$ angles ranging from 109.85 (4) to 115.98 (3)°. The mean $\text{Co}-\text{Cl}$ bond length, 2.27 (7) Å, is close to those observed in similar complexes (Zhang *et al.*, 2005).

There are $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen-bonding interactions between the cations and the anions (Table 2).

Experimental

Solutions of 2-aminopyridine and $\text{CoCl}_2\cdot 2\text{H}_2\text{O}$ in water were mixed in a 1:1 molar ratio and heated at 363 K for 2 h. Blue crystals of (I) were obtained by slow evaporation over a period of one week.

Crystal data

(C₅H₇N₂)₂[CoCl₄]
M_r = 390.98
 Monoclinic, C2/c
a = 8.2152 (3) Å
b = 14.0713 (5) Å
c = 13.5731 (5) Å
 β = 95.190 (2)°
V = 1562.52 (10) Å³

Z = 4
D_x = 1.662 Mg m⁻³
 Mo *K*α radiation
 μ = 1.77 mm⁻¹
T = 120 (2) K
 Block, blue
 0.4 × 0.25 × 0.2 mm

Data collection

Bruker–Nonius FR591 rotating-
 anode diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 SADABS (Sheldrick, 2003)
T_{min} = 0.595, *T_{max}* = 0.701
 8864 measured reflections

1801 independent reflections
 1488 reflections with *I* > 2σ(*I*)
R_{int} = 0.032
 θ_{\max} = 27.5°
 3 standard reflections
 every 60 reflections
 intensity decay: none

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.028
wR(*F*²) = 0.119
S = 1.26
 1801 reflections
 87 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.2962P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.57 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.67 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co—Cl2	2.2724 (7)	Co—Cl1	2.2755 (7)
C2—N1—C6	122.7 (2)	Cl2—Co—Cl2 ⁱ	109.85 (4)
Cl1—Co—Cl1 ⁱ	109.37 (4)	Cl2—Co—Cl1	115.98 (3)

Symmetry code: (i) $-x, y, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N7—H2A...Cl2 ⁱⁱ	0.86	2.42	3.258 (2)	165
N7—H2B...Cl1 ⁱⁱⁱ	0.86	2.44	3.286 (2)	169
N1—H1...Cl1 ^{iv}	0.86	2.58	3.275 (2)	139

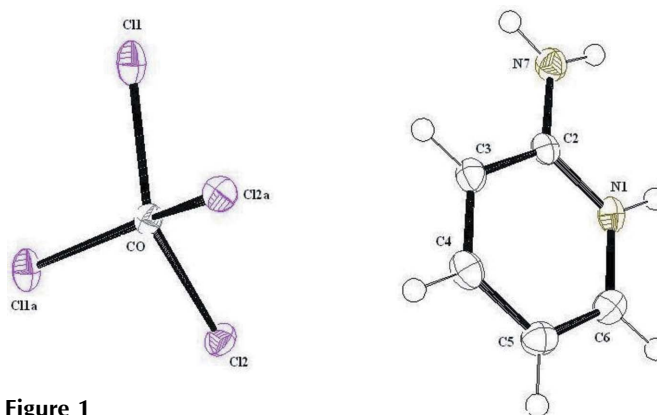
Symmetry codes: (ii) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iii) $x, -y, z - \frac{1}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Figure 1

The structure of (I), showing the atom-numbering scheme, with 50% probability displacement ellipsoids. The suffix *a* indicates the symmetry position $(-x, y, \frac{3}{2} - z)$.

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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