Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-aminopyridinium) tetrachlorocobalt(II)

Samuel Robinson Jebas,[a] Thailampillai Balasubramanian[b]* and Mark E Light[c]

[a]Department of Electronics, St Joseph's College, Tiruchirappalli 620002, India, [b]Department of Physics, National Institute of Technology, Tiruchirappalli 620015, India, and [c]School of Chemistry, University of Southampton, Highfield, SO17 1BJ, England

Correspondence e-mail: bala@nitt.edu

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.119
Data-to-parameter ratio = 20.7

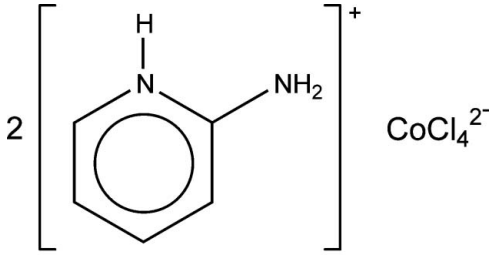
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 July 2006
Accepted 6 July 2006.

In the crystal structure of the title compound, $(C_5H_7N_2)_2[CoCl_4]$, 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 N—H···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).



(I)

The asymmetric unit of (I) contains a 2-aminopyridinium cation and half of a $[CoCl_4]^{2-}$ 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 C2—N1—C6 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 Cl—Co—Cl angles ranging from 109.85 (4) to 115.98 (3)° . The mean Co—Cl bond length, 2.27 (7) Å, is close to those observed in similar complexes (Zhang *et al.*, 2005).

There are N—H···Cl hydrogen-bonding interactions between the cations and the anions (Table 2).

Experimental

Solutions of 2-aminopyridine and $CoCl_2·2H_2O$ 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

$(C_5H_7N_2)_2[CoCl_4]$
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) Å^3
Z = 4
D_x = 1.662 Mg m^{-3}
Mo $K\alpha$ 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 $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°
3 standard reflections
every 60 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 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 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e 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, °).

D—H···A	D—H	H···A	D···A	D—H···A
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) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

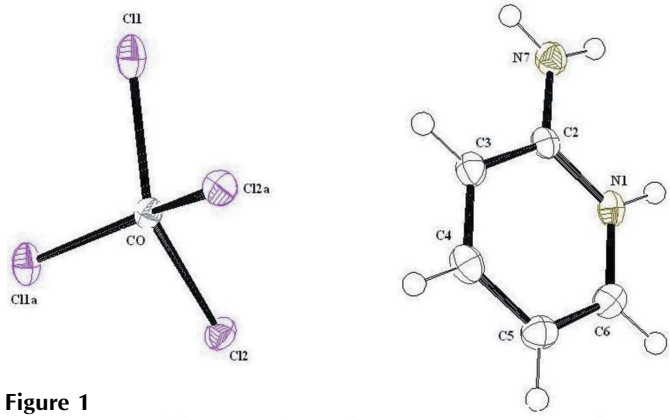


Figure 1
The structure of (I), showing the atom-numbering scheme, with 50% probability displacement ellipsoids. The suffix a indicates the symmetry position $(-x, y, \frac{3}{2}-z)$.

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_{iso}(H) = 1.2U_{eq}(C,*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).

References

Bis, J. A. & Zaworotko, M. J. (2005). *Cryst. Growth Des.* **5**, 1169–1179.
Chao, M., Schempp, E. & Rosenstein, R. D. (1975). *Acta Cryst.* B**31**, 2922–2924.
Jebas, S. R. & Balasubramanian, T. (2006). *Acta Cryst.* E**62**, o2209–o2211.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Smith, G., Bott, R. C. & Wermuth, U. D. (2000). *Acta Cryst.* C**56**, 1505–1506.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Windholz, M. (1976). The Merck Index. 9th Edition. Rahway, New Jersey, USA: Merck & Co., Inc.
Zhang, H., Fang, L. & Yuan, R. (2005). *Acta Cryst.* E**61**, m677–m678.