Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(pyridinium) tetrabromocobaltate(II)

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.015 Å
R factor = 0.061
wR factor = 0.157
Data-to-parameter ratio = 26.1

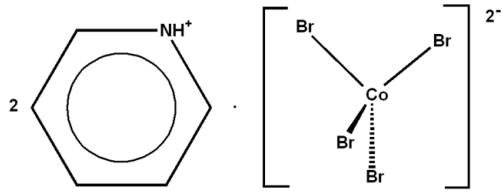
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $(C_5H_6N)_2[CoBr_4]$, contains discrete $[CoBr_4]^{2-}$ and pyridinium $C_5H_6N^+$ ions. Hydrogen bonds give rise to a three-dimensional network structure.

Received 21 February 2005
Accepted 22 February 2005
Online 26 February 2005

Comment

The pyridinium salt $(C_5H_6N)_2[CoCl_4]$, (II), which has a tetrachlorocobaltate(II) anion, has been described recently (Felloni *et al.*, 2004). In the title bis(pyridinium) tetrabromocobaltate analog, (I) (Fig. 1) tetrahedral $[CoBr_4]^{2-}$ anions and pyridinium $C_5H_6N^+$ cations are held together through N—H···Br hydrogen-bonding interactions (Table 2).



(I)

Experimental

An aqueous solution of HBr (10 ml, 4 *N*) was added to a mixture of cobalt(II) bromide hexahydrate (10 mmol) and pyridine (20 mmol) in

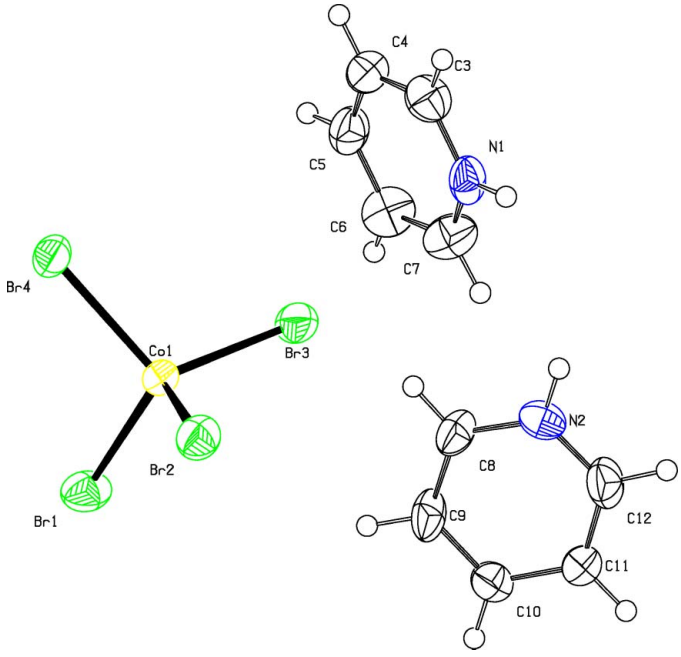


Figure 1
The molecular structure of (I), showing the atom numbering and displacement ellipsoids at the 50% probability level.

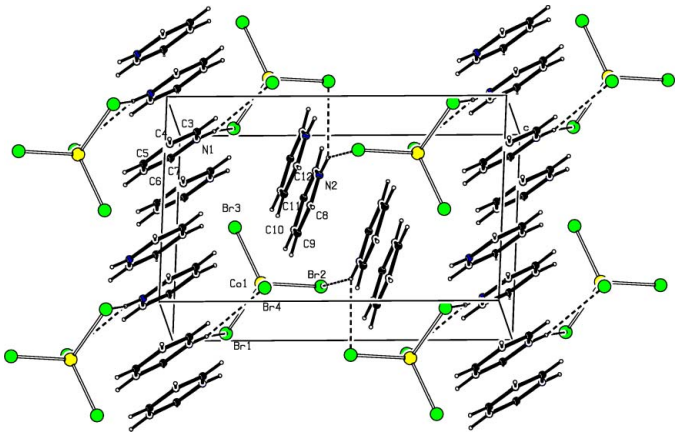


Figure 2
Packing of (I), with hydrogen bonds shown as dashed lines.

water (20 ml). The solution was allowed to evaporate at room temperature. After a few weeks, prism-shaped blue crystals of the title salt were obtained.

Crystal data

$(C_5H_6N)_2[CoBr_4]$
M_r = 538.79
Triclinic, $P\overline{1}$
a = 7.8331 (13) Å
b = 8.2205 (14) Å
c = 12.894 (2) Å
α = 88.237 (4)°
β = 83.013 (4)°
γ = 79.382 (3)°
V = 810.0 (2) Å^3
Z = 2
D_x = 2.209 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4026 reflections
θ = 1.6–28.3°
μ = 10.91 mm^{-1}
T = 223 (2) K
Prism, blue
0.18 × 0.16 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.15, T_{max} = 0.27
11355 measured reflections
4026 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 28.3°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.157
S = 0.99
4026 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 1.8493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—Br1	2.4080 (16)	Co1—Br3	2.3983 (16)
Co1—Br2	2.3937 (17)	Co1—Br4	2.4157 (16)
Br1—Co1—Br2	110.62 (6)	Br2—Co1—Br3	108.90 (6)
Br1—Co1—Br3	111.52 (6)	Br2—Co1—Br4	108.66 (6)
Br1—Co1—Br4	106.32 (6)	Br3—Co1—Br4	110.77 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Br1^{i}	0.87	2.71	3.417 (8)	140
N1—H1···Br4^{i}	0.87	2.89	3.527 (9)	132
N2—H2···Br2^{ii}	0.87	2.70	3.390 (8)	137
N2—H2···Br2^{i}	0.87	2.90	3.515 (8)	129

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

The H atoms were constrained to an ideal geometry, with C—H = 0.94 Å and N—H = 0.87 Å. All H atoms were refined with U_{iso}(H) = 1.2U_{eq}(parent atom). The maximum residual electron density is 0.86 Å from atom Br3 and the minimum electron density is 0.55 Å from Br2.

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: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

HZ thanks DAAD for a scholarship and Mr Klaus Kruse for the diffraction data collected at the diffraction facility at the Institute of Inorganic Chemistry, University of RWTH–Aachen.

References

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