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# Bis(imidazolium) tetrachlorocobaltate(II)

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**Key indicators**

Single-crystal X-ray study
*T* = 223 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.035
*wR* factor = 0.079
Data-to-parameter ratio = 24.3

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

The title compound, $(C_3H_5N_2)_2[CoCl_4]$, contains discrete $[CoCl_4]^{2-}$ anions and two imidazolium $C_3H_5N_2^+$ cations. Various N—H···Cl hydrogen bonds form a three-dimensional network.

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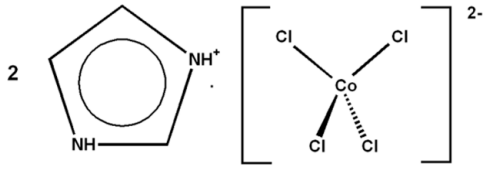
## Comment

A methylene-bridged bis(imidazolium) salt, $(C_9H_{14}N_4)[CoCl_4]$, containing a tetrachlorocobaltate(II) anion, has been described recently (Zeller *et al.*, 2005). In the related title compound, (I) (Fig. 1), tetrahedral $[CoCl_4]^{2-}$ anions and imidazolium cations are held together through N—H···Cl hydrogen-bonding interactions (Table 2), one of which, involving atom H1, is bifurcated.




(I)

## Experimental

An aqueous solution of HCl (20 ml, 2 *N*) was added to a mixture of cobalt(II) chloride hexahydrate (10 mmol) and imidazole (20 mmol) in water (20 ml). The solution was allowed to evaporate at room temperature and, after a few days, blue prismatic crystals of (I) were obtained.

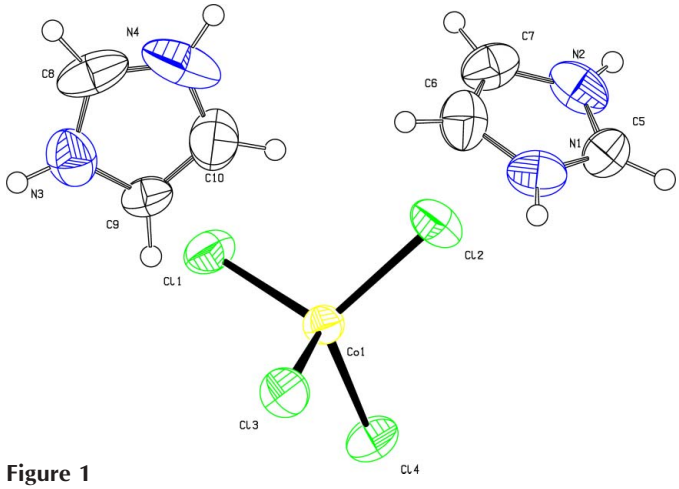



**Figure 1**
The molecular structure of (I), showing 50% displacement ellipsoids and arbitrary spheres for the H atoms.

*Crystal data*

$(C_3H_5N_2)_2[CoCl_4]$
$M_r$ = 338.91
Monoclinic, $P2_1/c$
$a$ = 7.686 (3) Å
$b$ = 13.498 (5) Å
$c$ = 12.808 (4) Å
$\beta$ = 93.138 (7)°
$V$ = 1326.7 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.697 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3299 reflections
$\theta$ = 2.2–28.3°
$\mu$ = 2.07 mm$^{-1}$
$T$ = 223 (2) K
Prism, blue
0.24 × 0.18 × 0.14 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.650, $T_{max}$ = 0.750
18064 measured reflections
3299 independent reflections
2236 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064
$\theta_{max}$ = 28.3°
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.079
$S$ = 0.89
3299 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co1—Cl1 | 2.2586 (8) | Co1—Cl3 | 2.2744 (8) |
| Co1—Cl2 | 2.2653 (8) | Co1—Cl4 | 2.2790 (8) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···Cl1$^{i}$ | 0.87 | 2.65 | 3.292 (2) | 132 |
| N1—H1···Cl4$^{ii}$ | 0.87 | 2.77 | 3.408 (2) | 132 |
| N2—H2···Cl2$^{iii}$ | 0.87 | 2.49 | 3.242 (3) | 145 |
| N3—H3···Cl3$^{iv}$ | 0.87 | 2.61 | 3.371 (3) | 147 |
| N4—H4···Cl4$^{v}$ | 0.87 | 2.37 | 3.215 (3) | 164 |

Symmetry codes: (i) $x-1, \frac{1}{2}-y, z-\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $1-x, 1-y, 1-z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (v) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$.

The H atoms were placed in idealized positions (C—H = 0.94 Å and N—H = 0.87 Å) and refined as riding with the constraint $U_{iso}(H) = 1.2U_{eq}(C,N)$.

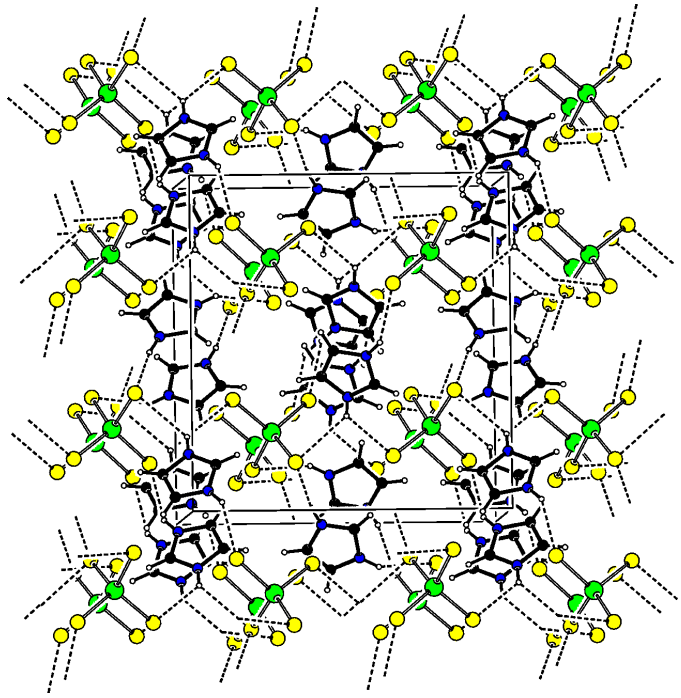


**Figure 2**
Packing diagram for (I), with hydrogen bonds shown as dashed lines. Colour key: Co green, Cl yellow, N blue, C black and H white.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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## References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zeller, A., Herdtweck, E. & Strassner, T. (2005), *Acta Cryst.* C**61**, m46–m47.