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Quinolinium trichloro(quinoline-*κN*)cobaltate(**II**)

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Key indicators

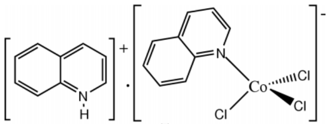
Single-crystal X-ray study
T = 295 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.079
Data-to-parameter ratio = 14.3

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

The title compound, $(C_9H_8N)[CoCl_3(C_9H_7N)]$, consists of Co^{II} complex anions and quinolinium cations. The Co^{II} complex anions assume tetrahedral coordination geometry and are hydrogen bonded to the quinolinium cations to form centrosymmetric supramolecular dimer. π–π stacking occurs between the quinoline and quinolinium rings.

Comment

π–π stacking between aromatic rings is correlated with the electron transfer processes in some biological systems (Deisenhofer & Michel, 1989). As part of our investigation of π–π stacking in metal complexes, a Co^{II} complex with a quinoline ligand has recently been prepared in the laboratory and its X-ray structure is presented here.



(I)

The structure of the title compound, (I), is shown in Fig. 1. (I) consists of Co^{II} complex anions and quinolinium cations. The Co^{II} complex anion assumes a distorted tetrahedral coordination geometry, formed by one quinoline molecule and three Cl atoms. The average Co—Cl bond distance of 2.2541 (8) Å (Table 1) is comparable to 2.2382 (17) Å found in the Cu^{II} analog (Savariault *et al.*, 1988) and 2.2513 (14) Å found in the Zn^{II} analog (Wang *et al.*, 2001), both determined at room temperature. The quinolinium cation links the neighboring Co^{II} complex anions *via* N—H$\cdots$Cl hydrogen bonding to form a centrosymmetric supramolecular dimer as shown in Fig. 1.

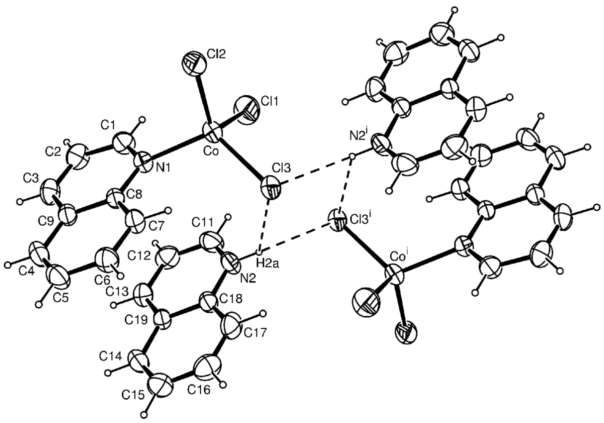


Figure 1
The structure of (I), with 30% probability displacement ellipsoids. Dashed lines show hydrogen bonds. [Symmetry code: (i) $1 - x$, $1 - y$, $1 - z$.]

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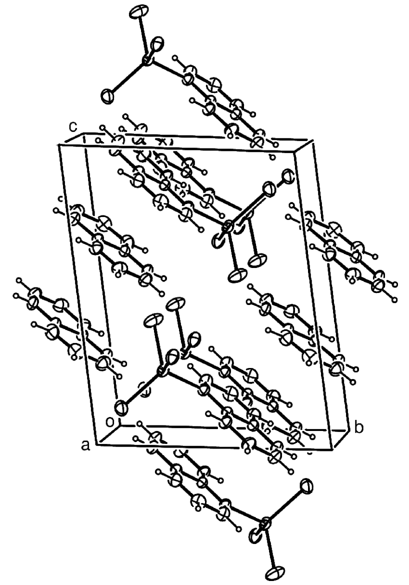

Figure 2
A molecular packing diagram showing the approximately parallel arrangement of quinoline and quinolinium rings.

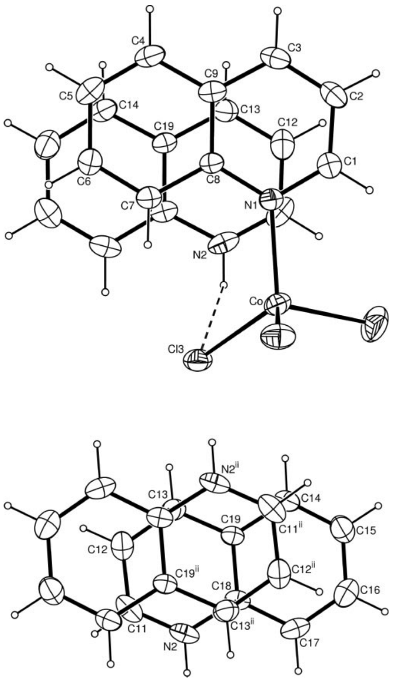

Figure 3
A diagram showing π–π stacking between quinoline and quinolinium rings (top) and between quinolinium rings (bottom). [Symmetry code: (ii) 1 $-x$, 2-y, 1-z.]

The molecular packing is illustrated in Fig. 2, showing the approximately parallel arrangement of quinoline and quinolinium rings in the crystal structure. The overlapped disposition of quinoline and quinolinium rings is illustrated in Fig. 3. The quinoline and quinolinium rings are nearly parallel, with a small dihedral angle of 3.52 (11)°, and the atoms C12, C13, C14 and C19 of the quinolinium are 3.513 (3), 3.566 (3), 3.658 (3) and 3.572 (2) Å, respectively, from the quinoline plane. The quinolinium cations related by an inversion centre are separated by 3.469 (4) Å. These findings suggest the existence of π–π stacking between quinoline and quinolinium rings and between quinolinium rings.

Experimental

An ethanol solution (15 ml) containing $CoCl_2\cdot 6H_2O$ (0.24 g, 1 mmol) and quinoline (0.26 g, 2 mmol) was mixed with an ethanol solution (10 ml) of succinic acid (0.12 g, 1 mmol) and Na_2CO_3 (0.11 g, 1 mmol). The solution was refluxed for 2 h and then filtered. Blue single crystals were obtained from the filtrate after 5 d.

Crystal data

$(C_9H_8N)[CoCl_3(C_9H_7N)]$
$M_r = 424.60$
Triclinic, $P\overline{1}$
$a = 8.2395$ (6) Å
$b = 9.4931$ (7) Å
$c = 11.9704$ (9) Å
$\alpha = 98.313$ (2)°
$\beta = 94.589$ (2)°
$\gamma = 106.191$ (3)°
$V = 882.56$ (11) Å^3

$Z = 2$
$D_x = 1.598$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5288 reflections
$\theta = 2.9$–24.0°
$\mu = 1.43$ mm^{-1}
$T = 295$ (2) K
Prism, blue
0.26 × 0.21 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.680$, $T_{\max} = 0.792$
6256 measured reflections

3100 independent reflections
2723 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 25.1°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.079$
$S = 1.07$
3100 reflections
217 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.5005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—N1	2.0643 (19)	Co—Cl1	2.2525 (8)
Co—Cl2	2.2375 (7)	Co—Cl3	2.2722 (7)
N1—Co—Cl2	106.12 (6)	N1—Co—Cl3	116.62 (6)
N1—Co—Cl1	103.13 (6)	Cl2—Co—Cl3	111.45 (3)
Cl2—Co—Cl1	114.55 (3)	Cl1—Co—Cl3	104.98 (3)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$a\cdots$Cl3	0.86	2.76	3.310 (2)	124
N2—H2$a\cdots$Cl3$^{\rm i}$	0.86	2.75	3.359 (2)	130

Symmetry code: (i) $1-x, 1-y, 1-z$.

H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å, and included in the final cycles of refinement in riding mode, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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