Monoclinic form of dichlorobis(quinoline-*N*)cobalt(II)

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In the structure of the title complex, $[CoCl_2(C_9H_7N)_2]$, the Co atom is coordinated by two chloride ligands and by two N atoms from two quinoline ligands. The geometry around the Co atom is slightly distorted tetrahedral, with Co—N bond lengths of 2.0697 (18) Å, Co—Cl bond lengths of 2.2445 (7) Å, and N—Co—N and Cl—Co—Cl bond angles of 107.16 (10) and 113.44 (4)°, respectively. The molecule has twofold rotation symmetry.

Comment

In view of the diverse structural types obtained with hindered nitrogen bases, a series of adducts of transition metal halides with monodentate nitrogen bases has been studied (Healy *et al.*, 1985; Savariault *et al.*, 1988). Our original object was to synthesize a heterometallic cobalt–manganese complex containing actetate and quinoline ligands, and the title compound, (I), was obtained. The complex exists in two forms: the monoclinic and the triclinic forms. The latter form was reported earlier (Golič & Mirčeva, 1988). The crystal structure of the compound consists of discrete neutral $[CoCl_2(C_9H_7N)_2]$ molecules, which lie on twofold axes. The molecular structure of the title complex is shown in Fig. 1. The packing diagram of the title compound is presented in Fig. 2. The Co atom is coordinated by two chloride ligands and two N atoms from two quinoline groups in a distorted tetrahedral arrangement. The N—Co—N, N—Co—Cl and Cl—Co—Cl bond angles are 107.16 (10), 102.56 (6) and 113.44 (4)°, respectively, with a Co—N bond length of 2.0697 (18) Å and a Co—Cl bond length of 2.2445 (7) Å, which are in good agreement with those found in other cobalt complexes (Clegg *et al.*, 1988; Long & Schlemper, 1975; Cui *et al.*, 1999).

(I)
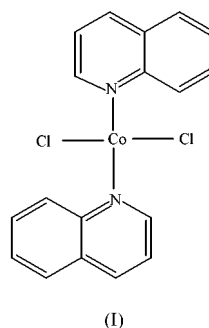
The molecular geometry within the quinoline ligands is normal (Mirčeva & Golič, 1990; Cui *et al.*, 2000). The quinoline ligands are planar, the maximum deviations of the atoms from the corresponding mean planes of the ligands being 0.0177 Å.
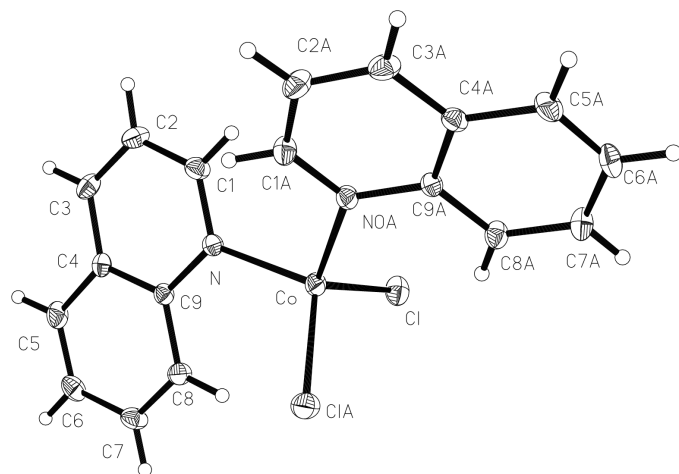
Figure 1
The structure of [CoCl₂(C₉H₇N)₂] showing the atom-numbering scheme (symmetry-equivalent atoms are labelled with the letter *A*) and displacement ellipsoids at the 30% probability level.

The dihedral angle formed by the two quinoline rings is 42.9 (3)°.

Experimental

Co(OAc)₂, MnCl₂.4H₂O and quinoline were mixed in ethanol and refluxed for 16 h; the resulting solution was allowed to stand at room temperature and purple crystals of the title complex were obtained after several weeks.

Crystal data

[CoCl₂(C₉H₇N)₂]	$D_x = 1.604$ Mg m^{-3}
$M_r = 388.14$	Mo $K\alpha$ radiation
Monoclinic, $P2/n$	Cell parameters from 2138
$a = 7.7864$ (8) Å	reflections
$b = 7.0874$ (7) Å	$\theta = 2.8–25.0°$
$c = 14.5616$ (15) Å	$\mu = 1.40$ mm^{-1}
$\beta = 90.174$ (2)°	$T = 293$ (2) K
$V = 803.58$ (14) Å^3	Plate, purple
$Z = 2$	$0.24 \times 0.18 \times 0.10$ mm
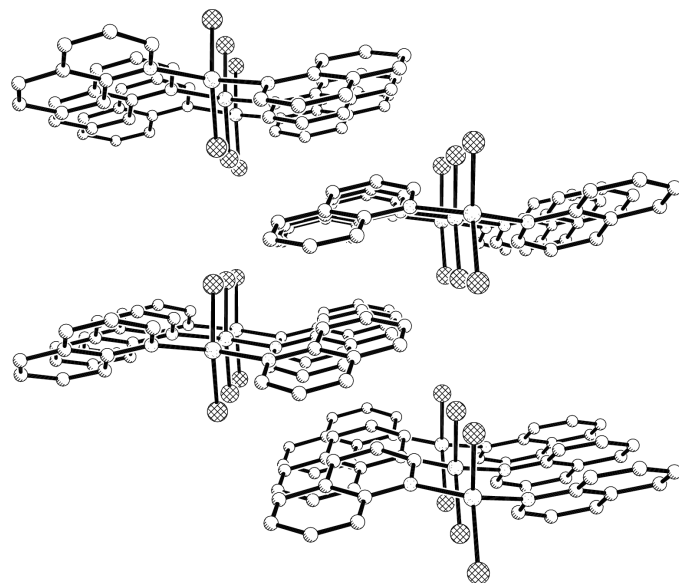
Figure 2
A packing diagram of the title compound viewed along the *b* axis.

Data collection

Siemens SMART CCD	1401 independent reflections
diffractometer	1202 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.020$
Absorption correction: empirical	$\theta_{max} = 25.0°$
(*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 9$
$T_{min} = 0.673$, $T_{max} = 0.869$	$k = -8 \rightarrow 7$
2782 measured reflections	$l = -13 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$+ 0.1707P]$
$wR(F^2) = 0.081$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.006$
1401 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
105 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co—N	2.0697 (18)	C1—C2	1.395 (4)
Co—Cl	2.2445 (7)	C2—C3	1.364 (4)
N—C1	1.329 (3)	C5—C4	1.421 (3)
N—C9	1.388 (3)	C7—C8	1.364 (3)
N—Co—N^i	107.16 (10)	C1—N—C9	117.4 (2)
N—Co—Cl	102.56 (6)	C1—N—Co	119.27 (16)
N^i—Co—Cl	115.72 (5)	C9—N—Co	123.23 (14)
N—Co—Cl^i	115.72 (5)	N—C1—C2	124.6 (2)
N^i—Co—Cl^i	102.56 (6)	N—C9—C4	121.0 (2)
Cl—Co—Cl^i	113.44 (4)	N—C9—C8	119.64 (19)

Symmetry code: (i) $\frac{1}{2} - x, y, \frac{1}{2} - z$.

H atoms were located from difference Fourier syntheses and included in the structure-factor calculations with a riding model.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SHELXTL XPREP* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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