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Dichlorobis(4-pyridone-κO)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.075
Data-to-parameter ratio = 17.5

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

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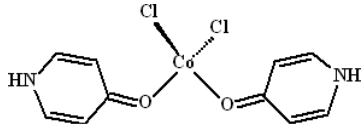
The Co atom in the title complex, $[CoCl_2(C_5H_5NO)_2]$, has a distorted tetrahedral coordination involving two Cl^- ions and two O atoms of two 4-pyridone ligands. The Co atom occupies a special position with twofold rotation symmetry. A layer structure is formed by N—H···Cl intermolecular hydrogen bonds and π–π stacking interactions of adjacent pyridone rings.

Comment

4-Hydroxypyridine has been widely used in pharmaceutical synthesis. It usually exists in equilibrium with the form 4-pyridone. However, in contrast to the metal complexes of 2-hydroxypyridine (Goodgame *et al.*, 1989; Blake *et al.*, 1991), there are few reports of structures of complexes of 4-hydroxypyridine or 4-pyridone (LaliaKantouri, 1996). Recently, we synthesized a cobalt complex of 4-pyridone, *viz.* dichlorobis(4-pyridone)cobalt(II), (I) (Fig. 1), by the reaction of 4-hydroxypyridine and $CoCl_2{\cdot}6H_2O$ in an ethanol solution. Compound (I) is isostructural with $[ZnCl_2(C_5H_5NO)_2]$ (Masse & Le Fur, 1998).



(I)

The Co atom in (I) exists in a tetrahedral coordination environment, defined by two Cl^- anions and two O atoms of 4-pyridone [Co—Cl = 2.2763 (8) Å and Co—O = 1.9550 (12) Å], and the Co atom occupies a special position with twofold rotation symmetry. The C1—C2, C4—C5 and C3—O1 bond lengths are 1.362 (2), 1.359 (3) and 1.2877 (19) Å, respectively. Interestingly, four N—H···Cl intermolecular hydrogen bonds generate a four-membered ring from four adjacent molecules. The four-membered ring has hydrogen-bonding distances (N···Cl) and angles (N—H···Cl) in the ranges 3.3481 (19)–

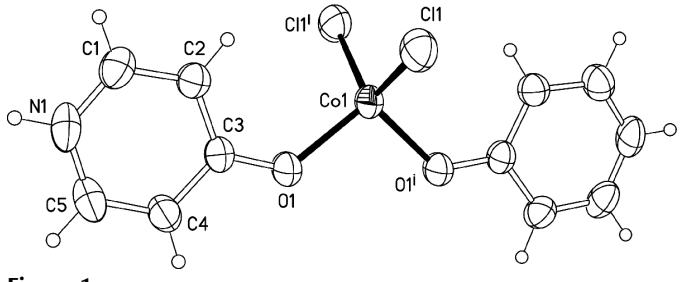


Figure 1
View of (I) with 50% probability ellipsoids. [Symmetry code: (i) $1-x, y, \frac{1}{2}-z$.]

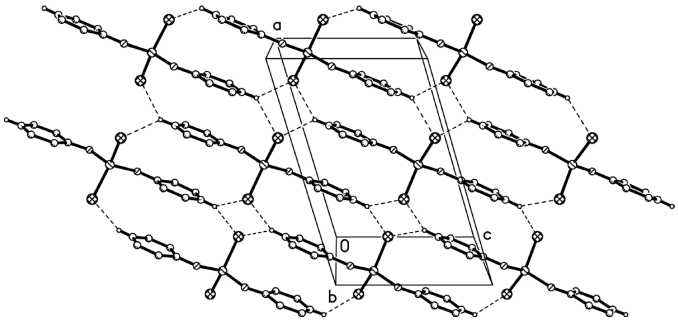


Figure 2
Packing diagram of (I), with hydrogen bonds indicated by dashed lines.

3.3574 (18) Å and 127 (2)–135 (2)°, respectively (Table 1). A two-dimensional layer structure is formed by these hydrogen bonds, and the Co···Co distances are 6.7933 (15) and 8.901 (2) Å. Furthermore, the layer architecture is stabilized by π–π interactions between adjacent pyridone ligands, with *Cg*···*Cg* (*Cg* is the centroid of the N1-containing ring) distances of 3.4429 (13) and 3.5372 (13) Å (Fig. 2).

Experimental

Compound (I) was prepared by the addition of $CoCl_2{\cdot}6H_2O$ (0.12 g, 0.5 mmol) to an ethanol solution of 4-hydroxypyridine (0.14 g, 1.5 mmol). The mixed solution was allowed to evaporate at room temperature and blue prism-shaped crystals were obtained after three days. Analysis calculated for $C_{10}H_{10}Cl_2CoN_2O_2$: C 37.53, H 3.15, N 8.75%; found: C 37.42, H 3.19, N 8.82%.

Crystal data

$[CoCl_2(C_5H_5NO)_2]$
M_r = 320.03
Monoclinic, $C2/c$
a = 13.185 (3) Å
b = 11.229 (2) Å
c = 8.7300 (17) Å
β = 106.70 (3)°
V = 1238.0 (5) Å^3
Z = 4
D_x = 1.717 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2929 reflections
θ = 3.1–27.5°
μ = 1.81 mm^{-1}
T = 293 (2) K
Prism, blue
0.36 × 0.24 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.551, T_{max} = 0.700
5774 measured reflections
1420 independent reflections
1323 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°
$h = -17 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.07
1420 reflections
81 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.7656P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H6···Cl1^{ii}	0.90 (3)	2.67 (2)	3.3574 (18)	135 (2)
N1—H6···Cl1^{iii}	0.90 (3)	2.74 (2)	3.3481 (19)	127 (2)

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

The H atom on the N atom was freely refined. The H atoms on C atoms were placed in calculated positions and treated as riding [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier atom)].

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

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