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Diaquabis(2-benzoylpyridine-$\kappa^2 N,O$)cobalt(II) bis(perchlorate)

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The reaction of 2-benzoylpyridine with cobalt(II) acetate tetrahydrate affords the mononuclear title compound, $[Co(C_{12}H_9NO)_2(H_2O)_2](ClO_4)_2$. The Co atom, which lies on an inversion centre, is six-coordinate in an octahedral geometry.

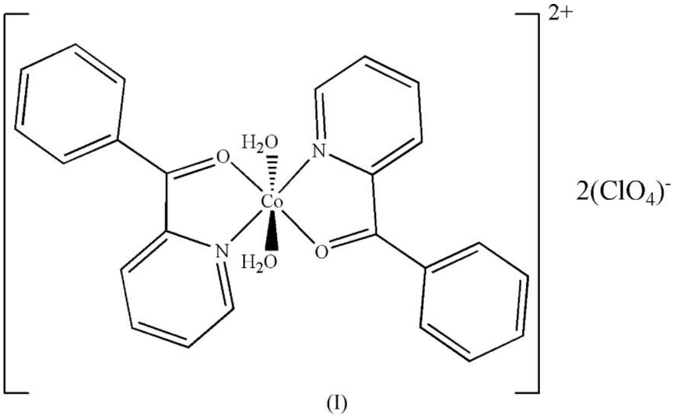
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.067
wR factor = 0.160
Data-to-parameter ratio = 12.5

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

Comment

2-Benzoylpyridine (bzpy) is a good chelating ligand. Some complexes based on bzpy have been isolated and structurally characterized (Schneider & Vahrenkamp, 2003; Milios *et al.*, 2004; Goher *et al.*, 1993, 1995, 1996; Mak & Goher, 1986; Mautner *et al.*, 1993; Abu-Youssef *et al.*, 1999; Zhang *et al.*, 2005; Sudbrake & Vahrenkamp, 2001). However, cobalt complexes of bzpy have never been reported. Here we report the synthesis and crystal structure of the title cobalt(II) complex, (I).



(I)

The crystal structure of (I) consists of $[Co(bzpy)_2(H_2O)_2]^{2+}$ cations and ClO_4^- anions (Fig. 1). In the cation, the Co^{II} atom, which lies on an inversion centre, shows an octahedral coordination provided by the N and O of two 2-benzoylpyridine ligands in the equatorial plane and by the O atoms of two water molecules in the axial positions. The Co—O and Co—N bond lengths range from 2.077 (5) to 2.105 (3) Å.

The crystal structure is stabilized by O—H···O hydrogen-bonding interactions (Table 1, Fig. 2) involving the coordinated water molecules and the O atoms of the perchlorate anions.

Experimental

The title complex was synthesized by refluxing a mixture of $Co(OAc)_2\cdot 4H_2O$ (1 mmol) and 2-benzoylpyridine (1 mmol) in ethanol/water (20 ml; 3:1 v/v) for 1 h at 373 K. After cooling, solid

$NaClO_4 \cdot H_2O$ (3 mmol) was added and the solution filtered. Red block-shaped crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of the filtrate over two weeks.

Crystal data

$[Co(C_{12}H_9NO)_2(H_2O)_2](ClO_4)_2$
$M_r = 660.27$
Monoclinic, $P2_1/n$
$a = 9.3598$ (5) Å
$b = 11.7387$ (6) Å
$c = 12.8062$ (7) Å
$\beta = 90.923$ (2)°
$V = 1406.86$ (13) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.87$ mm^{-1}
$T = 293$ (2) K
$0.10 \times 0.10 \times 0.08$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.818$, $T_{max} = 0.930$
4357 measured reflections
2434 independent reflections
1939 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.160$
$S = 1.16$
2434 reflections
195 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.75$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O6	0.85 (4)	1.89 (5)	2.742 (8)	176 (8)
O2—H2···O3^{i}	0.86 (4)	1.96 (5)	2.771 (7)	157 (8)

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

The H atoms of the water molecule were located in a difference Fourier synthesis and refined with an isotropic displacement parameter. All other H atoms were placed in idealized positions and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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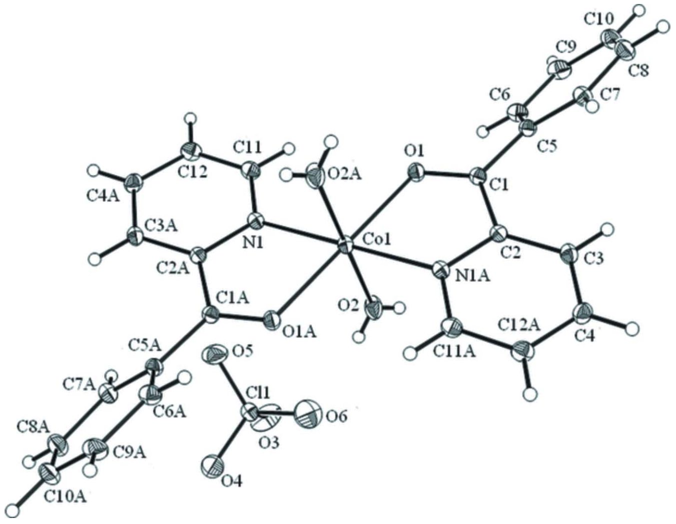

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. Atoms labelled with the suffix A are generated by the symmetry operation ($-x$, $1 - y$, $-z$).

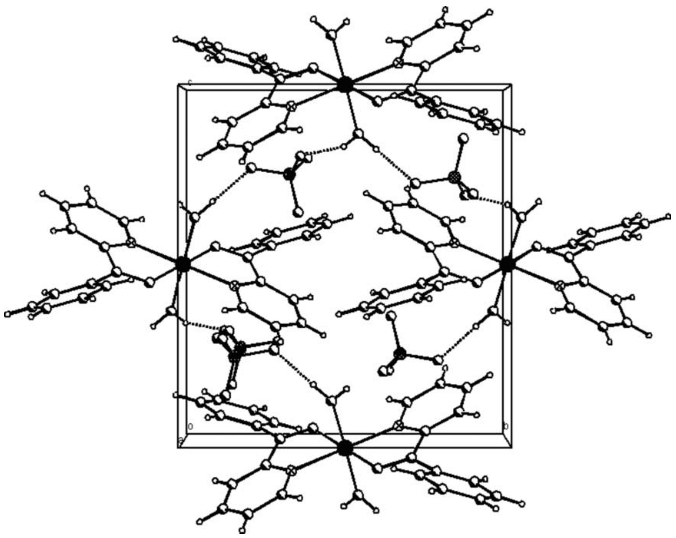

Figure 2
The molecular packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

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