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Bis(1-benzofuro[3,2-c]pyridine- κ N)-dichloridocobalt(II)Viktor Vrabel,^{a*} Ľubomír Švorc,^a Nadežda Juristová,^b Jozef Miklovič^b and Jozef Kožíšek^c^aInstitute of Analytical Chemistry, Faculty of Chemical and Food Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic,^bDepartment of Chemistry, Faculty of Natural Sciences, University of St Cyril and Methodius, 917 01 Trnava, Slovak Republic, and ^cInstitute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

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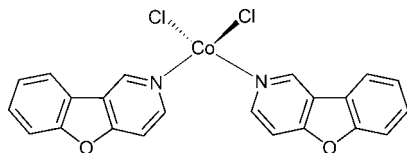
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.053; wR factor = 0.196; data-to-parameter ratio = 14.7.

In the title complex, $[\text{CoCl}_2(\text{C}_{11}\text{H}_7\text{NO})_2]$, the Co^{II} atom lies on a twofold rotation axis four-coordinated by two Cl atoms and two N-donor atoms from two 1-benzofuro[3,2-*c*]pyridine ligands, giving a slightly distorted tetrahedral coordination environment. The N/Co/N and Cl/Co/Cl planes are nearly perpendicular, with a dihedral angle of $87.1(1)^\circ$. The dihedral angle between the two benzofuro[3,2-*c*]pyridine ligands is $45.8(1)^\circ$. In the crystal structure, molecules are linked into a two-dimensional network parallel to the *ab* plane by $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Related literature

For ligand synthesis, see: Bobošík *et al.* (1995); Bencková & Krutošíková (1995, 1999). For general background, see: Baran *et al.* (2005); Billson *et al.* (2000); Fritsky *et al.* (2003); Jensen *et al.* (2000); Kotera *et al.* (2003); Lee & Wang (2007); Lumme *et al.* (1996); Masaki *et al.* (2002); Miklovič *et al.* (2004); Yang *et al.* (2006). For related structures, see: Amirnasr *et al.* (2002); Khalaji *et al.* (2006); Zhao *et al.* (2006).



Experimental

Crystal data

$[\text{CoCl}_2(\text{C}_{11}\text{H}_7\text{NO})_2]$
 $M_r = 468.21$
 Monoclinic, $C2/c$

$a = 7.7063(2)$ Å
 $b = 12.1886(3)$ Å
 $c = 20.4444(5)$ Å

$\beta = 96.217(3)^\circ$
 $V = 1909.03(8)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.20$ mm⁻¹
 $T = 298(2)$ K
 $0.38 \times 0.28 \times 0.03$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
 Absorption correction: analytical (Clark & Reid, 1995)
 $T_{\text{min}} = 0.698$, $T_{\text{max}} = 0.967$

15916 measured reflections
 1942 independent reflections
 1667 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.196$
 $S = 1.07$
 1942 reflections

132 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.97$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—Co1	2.033 (4)	Cl1—Co1	2.2259 (15)
N1 ⁱ —Co1—N1	115.3 (2)	N1—Co1—Cl1 ⁱ	103.65 (12)
N1—Co1—Cl1	108.07 (13)	Cl1—Co1—Cl1 ⁱ	118.59 (10)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2A\cdots\text{Cl}1^{\text{ii}}$	0.93	2.68	3.481 (6)	145

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2450).

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supplementary materials

Acta Cryst. (2007). E63, m2427-m2428 [doi:10.1107/S160053680704161X]

Bis(1-benzofuro[3,2-*c*]pyridine- κ N)dichloridocobalt(II)

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Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism and molecular architectures (Billson *et al.*, 2000; Fritsky *et al.*, 2003; Kotera *et al.*, 2003). Most of these compounds represent discrete mononuclear complexes (Masaki *et al.*, 2002; Khalaji *et al.*, 2006; Zhao *et al.*, 2006) but in some of them the Co atoms are connected into dinuclear units or polymers (Lumme *et al.*, 1996; Yang *et al.*, 2006; Jensen *et al.*, 2000; Lee & Wang, 2007). The furo[3,2-*c*]pyridine and its derivatives represent quinoline isosters, in which the benzene ring is replaced by the furan and pyridine ring can be readily coordinated to metal centers through N-donor atom (Miklovic *et al.*, 2004; Baran *et al.*, 2005). We report here the synthesis and crystal structure of the title compound, a mononuclear Co^{II} compound with a benzofuopyridine (BFP) ligand.

The Co^{II} atom lying on a twofold rotation axis is in a tetrahedral geometry and is coordinated by two BFP ligands and two chloride anions (Fig. 1). The Co—N [2.033 (4) Å] and Co—Cl [2.2259 (15) Å] bond lengths in the title compound are in good agreement with the corresponding mean distances in the related complexes (Amirnasr *et al.*, 2002; Zhao *et al.*, 2006; Khalaji *et al.*, 2006). The bond angles subtended at the Co1 atom range from 103.65 (12) to 118.59 (10)°, indicating a slightly distorted tetrahedral coordination. The dihedral angle between the nearly planar BFP ligands is 45.8 (1)°.

In the crystal structure of the title compound, C—H···Cl interactions (Table 2) involving atoms H2A and C11 connect the molecules into a two-dimensional network parallel to the *ab* plane. The formation of a four-coordinate complex, rather than a possible six-coordinate one, is attributed to the large volume of the monodentate BFP ligand.

Experimental

The organic ligand, [1]benzofuro[3,2-*c*]pyridine, was prepared according to literature procedures of Bobosik *et al.* (1995) and Benckova & Krutosikova (1995, 1999). To a CoCl₂·6H₂O (1 mmol) solution in ethanol (4 ml) was added the solution of [1]benzofuro[3,2-*c*]pyridine (3 mmol) in ethanol (4 ml) at room temperature. Small blue crystals were formed after 3 d. These were filtered off, washed with ethanol and recrystallized from tetrahydrofuran.

Refinement

All H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with C—H distances of 0.93 Å and U_{iso} set at 1.2 U_{eq} of the parent atom.

Figures

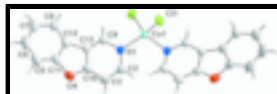


Fig. 1. The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x, y, 1/2 - z)$.

Bis(1-benzofuro[3,2-c]pyridine- κ N)dichloridocobalt(II)

Crystal data

$[\text{CoCl}_2(\text{C}_{11}\text{H}_7\text{NO})_2]$	$F_{000} = 948$
$M_r = 468.21$	$D_x = 1.629 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
Hall symbol: $-C 2yc$	$\lambda = 0.71073 \text{ \AA}$
$a = 7.7063 (2) \text{ \AA}$	Cell parameters from 8019 reflections
$b = 12.1886 (3) \text{ \AA}$	$\theta = 3.1\text{--}28.1^\circ$
$c = 20.4444 (5) \text{ \AA}$	$\mu = 1.20 \text{ mm}^{-1}$
$\beta = 96.217 (3)^\circ$	$T = 298 (2) \text{ K}$
$V = 1909.03 (8) \text{ \AA}^3$	Plate, blue
$Z = 4$	$0.38 \times 0.28 \times 0.03 \text{ mm}$

Data collection

Oxford Diffraction Gemini R CCD diffractometer	1942 independent reflections
Radiation source: fine-focus sealed tube	1667 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.030$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 26.4^\circ$
Rotation method data acquisition using ω and φ scans	$\theta_{\text{min}} = 4.1^\circ$
Absorption correction: analytical (Clark & Reid, 1995)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.698$, $T_{\text{max}} = 0.967$	$k = -15 \rightarrow 15$
15916 measured reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.196$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 12.9573P]$
$S = 1.07$	where $P = (F_o^2 + 2F_c^2)/3$
1942 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
132 parameters	$\Delta\rho_{\text{max}} = 0.97 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Experimental. face-indexed (*CrysAlis RED*; Oxford Diffraction, 2006)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C2	0.0900 (7)	0.1711 (5)	0.3404 (3)	0.0465 (12)
H2A	0.1235	0.1378	0.3028	0.056*
C3	0.1133 (8)	0.1134 (5)	0.3987 (3)	0.0505 (13)
H3A	0.1587	0.0426	0.4010	0.061*
C5	-0.0026 (9)	0.2030 (6)	0.6201 (3)	0.0629 (18)
H5A	0.0322	0.1409	0.6445	0.076*
C6	-0.0707 (9)	0.2930 (7)	0.6481 (3)	0.067 (2)
H6A	-0.0807	0.2924	0.6930	0.080*
C7	-0.1249 (9)	0.3847 (6)	0.6118 (3)	0.0609 (17)
H7A	-0.1717	0.4439	0.6326	0.073*
C8	-0.1110 (7)	0.3902 (5)	0.5448 (3)	0.0484 (13)
H8A	-0.1472	0.4521	0.5205	0.058*
C9	-0.0246 (7)	0.3226 (4)	0.3884 (2)	0.0390 (11)
H9A	-0.0718	0.3928	0.3847	0.047*
C10	0.0656 (7)	0.1663 (4)	0.4527 (3)	0.0418 (11)
C11	0.0114 (7)	0.2096 (5)	0.5533 (3)	0.0471 (13)
C12	-0.0411 (7)	0.3001 (4)	0.5151 (2)	0.0418 (12)
C13	-0.0044 (6)	0.2728 (4)	0.4488 (2)	0.0359 (10)
N1	0.0219 (6)	0.2728 (3)	0.33452 (19)	0.0388 (9)
O4	0.0769 (6)	0.1264 (3)	0.51576 (19)	0.0527 (10)
Cl1	0.2471 (2)	0.45525 (13)	0.24621 (7)	0.0552 (4)
Co1	0.0000	0.36200 (8)	0.2500	0.0387 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.051 (3)	0.043 (3)	0.047 (3)	0.006 (2)	0.014 (2)	-0.003 (2)
C3	0.057 (3)	0.037 (3)	0.057 (3)	0.011 (2)	0.003 (3)	0.002 (2)
C5	0.070 (4)	0.081 (5)	0.037 (3)	-0.022 (4)	-0.003 (3)	0.018 (3)
C6	0.071 (4)	0.100 (6)	0.029 (3)	-0.031 (4)	0.005 (3)	-0.004 (3)
C7	0.066 (4)	0.074 (4)	0.046 (3)	-0.021 (3)	0.016 (3)	-0.016 (3)
C8	0.050 (3)	0.055 (3)	0.041 (3)	-0.011 (3)	0.010 (2)	-0.008 (2)
C9	0.044 (3)	0.037 (2)	0.037 (2)	0.000 (2)	0.008 (2)	0.001 (2)
C10	0.041 (3)	0.041 (3)	0.042 (3)	0.000 (2)	-0.001 (2)	0.008 (2)
C11	0.052 (3)	0.053 (3)	0.036 (3)	-0.013 (2)	0.000 (2)	0.007 (2)
C12	0.045 (3)	0.050 (3)	0.031 (2)	-0.010 (2)	0.004 (2)	0.003 (2)
C13	0.039 (2)	0.035 (2)	0.034 (2)	-0.005 (2)	0.0050 (19)	0.0010 (19)
N1	0.045 (2)	0.039 (2)	0.034 (2)	0.0006 (18)	0.0096 (17)	0.0008 (17)
O4	0.063 (3)	0.048 (2)	0.044 (2)	0.0023 (19)	-0.0042 (18)	0.0157 (17)
Cl1	0.0641 (9)	0.0577 (9)	0.0452 (7)	-0.0172 (7)	0.0122 (6)	0.0013 (6)
Co1	0.0484 (6)	0.0396 (6)	0.0298 (5)	0.000	0.0116 (4)	0.000

Geometric parameters (\AA , $^\circ$)

C2—N1	1.346 (7)	C8—H8A	0.93
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supplementary materials

C2—C3	1.379 (8)	C9—N1	1.340 (6)
C2—H2A	0.93	C9—C13	1.369 (7)
C3—C10	1.362 (8)	C9—H9A	0.93
C3—H3A	0.93	C10—O4	1.373 (6)
C5—C6	1.368 (11)	C10—C13	1.405 (7)
C5—C11	1.384 (8)	C11—C12	1.385 (7)
C5—H5A	0.93	C11—O4	1.397 (7)
C6—C7	1.382 (11)	C12—C13	1.454 (7)
C6—H6A	0.93	N1—Co1	2.033 (4)
C7—C8	1.386 (8)	Cl1—Co1	2.2259 (15)
C7—H7A	0.93	Co1—N1 ⁱ	2.033 (4)
C8—C12	1.391 (8)	Co1—Cl1 ⁱ	2.2259 (15)
N1—C2—C3	124.0 (5)	C3—C10—C13	121.8 (5)
N1—C2—H2A	118.0	O4—C10—C13	111.4 (5)
C3—C2—H2A	118.0	C5—C11—C12	123.5 (6)
C10—C3—C2	115.9 (5)	C5—C11—O4	124.8 (6)
C10—C3—H3A	122.0	C12—C11—O4	111.7 (4)
C2—C3—H3A	122.0	C11—C12—C8	119.1 (5)
C6—C5—C11	116.2 (6)	C11—C12—C13	105.6 (5)
C6—C5—H5A	121.9	C8—C12—C13	135.3 (5)
C11—C5—H5A	121.9	C9—C13—C10	117.7 (5)
C5—C6—C7	122.0 (6)	C9—C13—C12	136.5 (5)
C5—C6—H6A	119.0	C10—C13—C12	105.7 (4)
C7—C6—H6A	119.0	C9—N1—C2	118.7 (4)
C6—C7—C8	121.3 (6)	C9—N1—Co1	116.8 (3)
C6—C7—H7A	119.4	C2—N1—Co1	124.3 (3)
C8—C7—H7A	119.4	C10—O4—C11	105.6 (4)
C7—C8—C12	117.9 (6)	N1 ⁱ —Co1—N1	115.3 (2)
C7—C8—H8A	121.0	N1 ⁱ —Co1—Cl1	103.65 (12)
C12—C8—H8A	121.0	N1—Co1—Cl1	108.07 (13)
N1—C9—C13	121.8 (5)	N1 ⁱ —Co1—Cl1 ⁱ	108.07 (13)
N1—C9—H9A	119.1	N1—Co1—Cl1 ⁱ	103.65 (12)
C13—C9—H9A	119.1	Cl1—Co1—Cl1 ⁱ	118.59 (10)
C3—C10—O4	126.8 (5)		
N1—C2—C3—C10	-1.3 (9)	O4—C10—C13—C12	-0.7 (6)
C11—C5—C6—C7	1.0 (10)	C11—C12—C13—C9	179.2 (6)
C5—C6—C7—C8	-0.7 (10)	C8—C12—C13—C9	-1.0 (11)
C6—C7—C8—C12	0.3 (9)	C11—C12—C13—C10	0.8 (6)
C2—C3—C10—O4	-179.7 (5)	C8—C12—C13—C10	-179.4 (6)
C2—C3—C10—C13	0.6 (8)	C13—C9—N1—C2	0.0 (8)
C6—C5—C11—C12	-0.8 (9)	C13—C9—N1—Co1	-175.6 (4)
C6—C5—C11—O4	-179.8 (6)	C3—C2—N1—C9	1.0 (8)
C5—C11—C12—C8	0.4 (8)	C3—C2—N1—Co1	176.3 (4)
O4—C11—C12—C8	179.5 (5)	C3—C10—O4—C11	-179.5 (6)
C5—C11—C12—C13	-179.8 (5)	C13—C10—O4—C11	0.3 (6)
O4—C11—C12—C13	-0.7 (6)	C5—C11—O4—C10	179.3 (5)
C7—C8—C12—C11	-0.1 (8)	C12—C11—O4—C10	0.3 (6)

C7—C8—C12—C13	-179.8 (6)	C9—N1—Co1—N1 ⁱ	-157.1 (4)
N1—C9—C13—C10	-0.6 (7)	C2—N1—Co1—N1 ⁱ	27.5 (4)
N1—C9—C13—C12	-178.9 (5)	C9—N1—Co1—C11	87.5 (4)
C3—C10—C13—C9	0.3 (8)	C2—N1—Co1—C11	-87.9 (4)
O4—C10—C13—C9	-179.4 (4)	C9—N1—Co1—C11 ⁱ	-39.2 (4)
C3—C10—C13—C12	179.1 (5)	C2—N1—Co1—C11 ⁱ	145.4 (4)

Symmetry codes: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2A \cdots C11 ⁱⁱ	0.93	2.68	3.481 (6)	145

Symmetry codes: (ii) $-x+1/2, y-1/2, -z+1/2$.

Fig. 1

