

Diaquabis(4-formylbenzoato- κ O¹)bis-(nicotinamide- κ N¹)cobalt(II)

Mustafa Sertçelik,^a Nagihan Çaylak Delibaş,^b Hacali Necefoğlu^a and Tuncer Hökelek^{c*}

^aDepartment of Chemistry, Kafkas University, 36100 Kars, Turkey, ^bDepartment of Physics, Sakarya University, 54187 Esentepe, Sakarya, Turkey, and ^cDepartment of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey

Correspondence e-mail: merzifon@hacettepe.edu.tr

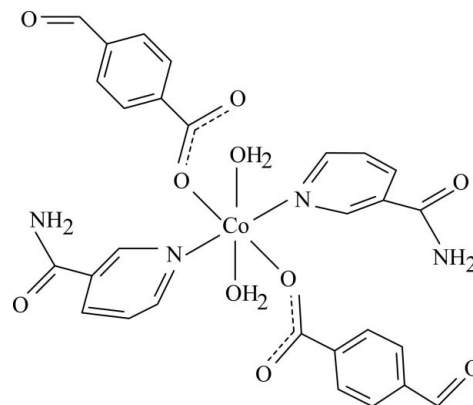
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.026; wR factor = 0.069; data-to-parameter ratio = 16.3.

In the title complex, $[\text{Co}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$, the Co^{II} cation is located on an inversion center and is coordinated by two 4-formylbenzoate (FB) anions, two nicotinamide (NA) ligands and two water molecules. The four O atoms in the equatorial plane around the Co^{II} cation form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands in the axial positions. The dihedral angle between the carboxylate group and the adjacent benzene ring is $23.91(9)^\circ$, while the pyridine and benzene rings are oriented at a dihedral angle of $88.84(4)^\circ$. The coordinating water molecule links with the carboxylate group *via* an intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond. In the crystal, $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$ and weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into a three-dimensional supra-molecular network. $\pi-\pi$ stacking between the parallel benzene rings of adjacent molecules [centroid-centroid distance = $3.8505(8)$ Å] may further stabilize the structure. A weak $\text{C}-\text{H}\cdots\pi$ interaction also occurs in the crystal.

Related literature

For literature on niacin, see: Krishnamachari (1974). For information on the nicotinic acid derivative *N,N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Aydın *et al.* (2012); Hökelek *et al.* (1996, 2009*a,b*); Hökelek & Necefoğlu (1998, 2007); Necefoğlu *et al.* (2011*a,b*); Sertçelik *et al.* (2012*a,b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Co}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$
 $M_r = 637.46$
 Triclinic, $P\bar{1}$
 $a = 7.7784(2)$ Å
 $b = 9.7988(3)$ Å
 $c = 9.8970(3)$ Å
 $\alpha = 78.080(3)^\circ$
 $\beta = 71.395(2)^\circ$
 $\gamma = 86.638(4)^\circ$
 $V = 699.48(4)$ Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.68$ mm⁻¹
 $T = 100$ K
 $0.33 \times 0.17 \times 0.10$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\text{min}} = 0.808$, $T_{\text{max}} = 0.937$
 12735 measured reflections
 3527 independent reflections
 3301 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.069$
 $S = 1.05$
 3527 reflections
 216 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the pyridine ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H21}\cdots\text{O2}^{\text{i}}$	0.87 (2)	2.078 (19)	2.8834 (15)	153 (2)
$\text{N2}-\text{H22}\cdots\text{O4}^{\text{ii}}$	0.86 (2)	2.04 (2)	2.8908 (16)	167 (2)
$\text{O5}-\text{H51}\cdots\text{O4}^{\text{iii}}$	0.81 (2)	2.08 (2)	2.8583 (13)	162.3 (19)
$\text{O5}-\text{H52}\cdots\text{O2}^{\text{iv}}$	0.87 (2)	1.83 (2)	2.6774 (14)	164 (2)
$\text{C6}-\text{H6}\cdots\text{O2}^{\text{iii}}$	0.93	2.39	3.3123 (17)	172
$\text{C13}-\text{H13}\cdots\text{O3}^{\text{v}}$	0.93	2.47	3.3120 (18)	150
$\text{C4}-\text{H4}\cdots\text{C}_g^{\text{vi}}$	0.93	2.72	3.6338 (14)	167

Symmetry codes: (i) $x, y, z - 1$; (ii) $-x - 1, -y, -z - 1$; (iii) $x + 1, y, z$; (iv) $-x, -y, -z$; (v) $-x + 1, -y + 1, -z$; (vi) $-x, -y + 1, -z + 2$.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5597).

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supporting information

Acta Cryst. (2012). E68, m1091–m1092 [https://doi.org/10.1107/S1600536812032205]

Diaquabis(4-formylbenzoato- κO^1)bis(nicotinamide- κN^1)cobalt(II)

Mustafa Sertçelik, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek

S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N,N*-diethylnicotinamide (DNA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

In the title mononuclear complex, Co^{II} cation is located on an inversion center and is coordinated by two 4-formylbenzoate (FB) anions, two nicotinamide (NA) ligands and two water molecules, all ligands coordinating in a monodentate manner (Fig. 1). The crystal structures of similar complexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions, [Cu(C₇H₅O₂)₂(C₁₀H₁₄N₂O)₂] (Hökelek *et al.*, 1996), [Cu(C₇H₄BrO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Necefoğlu *et al.*, 2011a), [Co(C₆H₆N₂O)₂(C₇H₄NO₄)₂(H₂O)₂] (Hökelek & Necefoğlu, 1998), [Co(C₉H₉O₂)₂(C₁₀H₁₄N₂O)₂(H₂O)₂] (Necefoğlu *et al.*, 2011b), [Co(C₇H₄IO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Aydın *et al.*, 2012), [Ni(C₇H₄ClO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Hökelek *et al.*, 2009a), [Ni(C₅H₅O₃)₂(C₆H₆N₂O)₂(H₂O)₂] (Sertçelik *et al.*, 2012a), [Mn(C₉H₁₀NO₂)₂(H₂O)₄].2H₂O (Hökelek & Necefoğlu, 2007), [Zn(C₇H₄BrO₂)₂(C₆H₆N₂O)₂(H₂O)₂] (Hökelek *et al.*, 2009b) and [Zn(C₈H₅O₃)₂(C₁₀H₁₄N₂O)₂(H₂O)₂] (Sertçelik *et al.*, 2012b) have also been reported. In the copper(II) complex mentioned above the two benzoate ions coordinate to the Cu^{II} atom as bidentate ligands, while in the other structures all the ligands coordinate in a monodentate manner.

In the title complex, the four symmetry related O atoms (O1, O1', O5 and O5') in the equatorial plane around the Co^{II} ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two symmetry related N atoms of the NA ligands (N1 and N1') in the axial positions. The near equalities of the C1—O1 [1.2610 (14) Å] and C1—O2 [1.2608 (15) Å] bonds in the carboxylate group indicate delocalized bonding arrangement, rather than localized single and double bonds. The Co—O bond lengths are 2.0864 (8) Å (for benzoate oxygens) and 2.1254 (9) Å (for water oxygens), and the Co—N bond length is 2.1276 (10) Å, close to standard values (Allen *et al.*, 1987). The Co atom is displaced out of the mean-plane of the carboxylate group (O1/C1/O2) by -0.5901 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring A (C2—C7) is 23.91 (9)°. The benzene A (C2—C7) and the pyridine B (N1/C9—C13) rings are oriented at a dihedral angle of A/B = 88.84 (4)°. The coordinating water molecule links with the carboxylate group *via* an O—H...O hydrogen bond (Table 1).

In the crystal, intermolecular N—H...O, O—H...O and weak C—H...O hydrogen bonds (Table 1) link the molecules into a three-dimensional supramolecular network, in which they may be effective in the stabilization of the structure. The $\pi\cdots\pi$ contact between the benzene rings, Cg1—Cg1ⁱ [symmetry code: (i) 1 - x, 1 - y, 2 - z, where Cg1 is the centroid of the ring A (C2—C7)] may further stabilize the structure, with centroid-centroid distance of 3.8505 (8) Å. A weak C-H... π interaction also occurs in the crystal.

S2. Experimental

The title compound was prepared by the reaction of CoSO₄·H₂O (0.865 g, 5 mmol) in H₂O (25 ml) and NA (1.22 g, 50 mmol) in H₂O (100 ml) with sodium 4-formylbenzoate (1.72 g, 10 mmol) in H₂O (100 ml) at room temperature. The

mixture was filtered and set aside to crystallize at ambient temperature for several days, giving orange single crystals.

S3. Refinement

Atoms H8 (for CH), H21 and H22 (for NH₂) and H51 and H52 (for H₂O) were located in a difference Fourier map and were refined freely. The C-bound H-atoms were positioned geometrically with C—H = 0.93 Å for aromatic H-atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

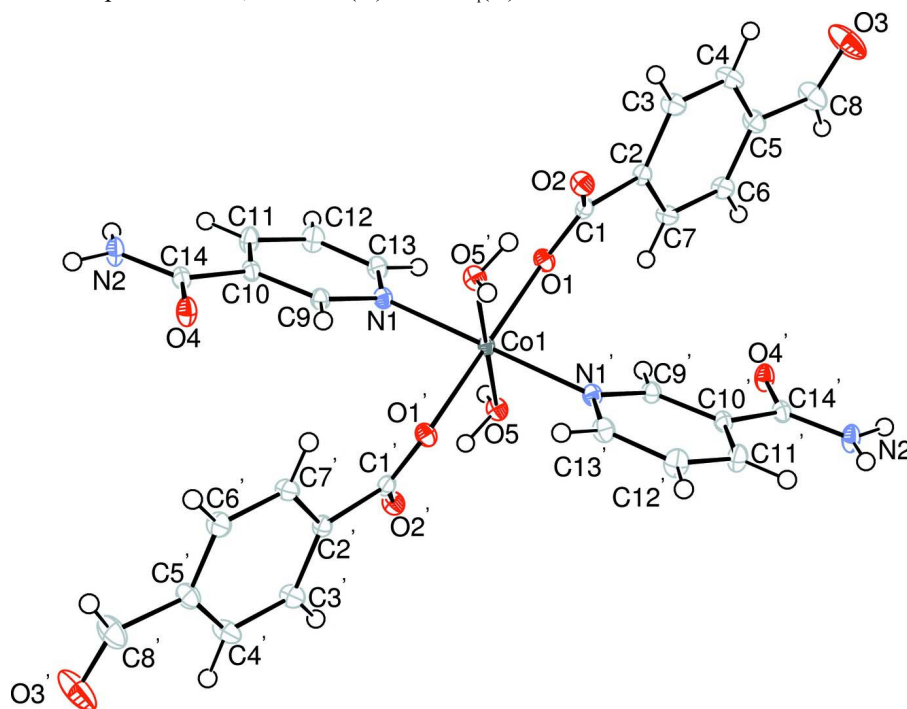


Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (') -x, -y, -z].

Diaquabis(4-formylbenzoato- κO^1)bis(nicotinamide- κN^1)cobalt(II)

Crystal data

[Co(C₈H₅O₃)₂(C₆H₆N₂O)₂(H₂O)₂]

$M_r = 637.46$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7784$ (2) Å

$b = 9.7988$ (3) Å

$c = 9.8970$ (3) Å

$\alpha = 78.080$ (3)°

$\beta = 71.395$ (2)°

$\gamma = 86.638$ (4)°

$V = 699.48$ (4) Å³

$Z = 1$

$F(000) = 329$

$D_x = 1.513$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7533 reflections

$\theta = 2.8$ – 28.5 °

$\mu = 0.68$ mm⁻¹

$T = 100$ K

Block, orange

$0.33 \times 0.17 \times 0.10$ mm

Data collection

Bruker Kappa APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator
 φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.808$, $T_{\max} = 0.937$

12735 measured reflections

3527 independent reflections

3301 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 28.5^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.069$

$S = 1.05$

3527 reflections

216 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.3387P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.0000	0.01057 (7)
O1	0.12202 (11)	0.18006 (9)	0.01007 (10)	0.01452 (18)
O2	-0.11185 (12)	0.27803 (9)	0.15705 (10)	0.01572 (18)
O3	0.49561 (15)	0.66922 (13)	0.31971 (16)	0.0403 (3)
O4	-0.43334 (12)	0.00199 (10)	-0.33497 (10)	0.01763 (19)
O5	0.26433 (12)	-0.08141 (10)	-0.07947 (10)	0.01505 (18)
H51	0.345 (3)	-0.041 (2)	-0.147 (2)	0.029 (5)*
H52	0.236 (3)	-0.151 (2)	-0.110 (2)	0.040 (5)*
N1	-0.00257 (14)	0.09276 (10)	-0.21360 (11)	0.0129 (2)
N2	-0.32789 (16)	0.13287 (12)	-0.56018 (12)	0.0176 (2)
H21	-0.244 (3)	0.1859 (19)	-0.628 (2)	0.028 (5)*
H22	-0.413 (3)	0.1007 (19)	-0.584 (2)	0.029 (5)*
C1	0.05487 (16)	0.26423 (12)	0.09348 (13)	0.0123 (2)
C2	0.18468 (16)	0.35171 (12)	0.12577 (13)	0.0126 (2)
C3	0.12393 (17)	0.47283 (13)	0.18014 (14)	0.0168 (2)
H3	0.0067	0.5042	0.1877	0.020*
C4	0.23769 (17)	0.54602 (13)	0.22256 (15)	0.0192 (3)
H4	0.1976	0.6270	0.2579	0.023*

C5	0.41275 (17)	0.49803 (13)	0.21208 (14)	0.0170 (2)
C6	0.47496 (17)	0.37952 (13)	0.15538 (14)	0.0166 (2)
H6	0.5927	0.3489	0.1469	0.020*
C7	0.36129 (16)	0.30652 (12)	0.11124 (14)	0.0150 (2)
H7	0.4033	0.2278	0.0721	0.018*
C8	0.53655 (19)	0.57111 (16)	0.26075 (18)	0.0256 (3)
H8	0.658 (2)	0.5327 (18)	0.2431 (19)	0.026 (4)*
C9	-0.14389 (16)	0.06886 (12)	-0.25570 (13)	0.0130 (2)
H9	-0.2389	0.0133	-0.1891	0.016*
C10	-0.15532 (16)	0.12280 (12)	-0.39347 (13)	0.0128 (2)
C11	-0.01388 (18)	0.20716 (14)	-0.49194 (14)	0.0174 (2)
H11	-0.0172	0.2454	-0.5852	0.021*
C12	0.13220 (18)	0.23343 (14)	-0.44905 (14)	0.0188 (3)
H12	0.2279	0.2900	-0.5130	0.023*
C13	0.13331 (16)	0.17428 (13)	-0.30981 (14)	0.0152 (2)
H13	0.2319	0.1916	-0.2817	0.018*
C14	-0.31771 (16)	0.08278 (12)	-0.42778 (13)	0.0138 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00908 (11)	0.01327 (11)	0.01077 (12)	-0.00042 (8)	-0.00433 (8)	-0.00344 (8)
O1	0.0133 (4)	0.0159 (4)	0.0150 (4)	-0.0020 (3)	-0.0039 (3)	-0.0047 (3)
O2	0.0111 (4)	0.0182 (4)	0.0186 (4)	-0.0011 (3)	-0.0045 (3)	-0.0052 (3)
O3	0.0230 (6)	0.0454 (7)	0.0642 (9)	-0.0011 (5)	-0.0124 (6)	-0.0386 (7)
O4	0.0163 (4)	0.0237 (5)	0.0137 (4)	-0.0062 (3)	-0.0062 (3)	-0.0015 (3)
O5	0.0115 (4)	0.0177 (4)	0.0162 (4)	-0.0009 (3)	-0.0036 (4)	-0.0048 (4)
N1	0.0123 (5)	0.0144 (5)	0.0136 (5)	-0.0006 (4)	-0.0053 (4)	-0.0036 (4)
N2	0.0176 (5)	0.0237 (6)	0.0132 (5)	-0.0058 (4)	-0.0077 (4)	-0.0014 (4)
C1	0.0131 (5)	0.0124 (5)	0.0116 (5)	-0.0020 (4)	-0.0058 (4)	0.0006 (4)
C2	0.0119 (5)	0.0136 (5)	0.0122 (5)	-0.0022 (4)	-0.0043 (4)	-0.0011 (4)
C3	0.0116 (5)	0.0168 (6)	0.0225 (6)	0.0009 (4)	-0.0050 (5)	-0.0058 (5)
C4	0.0150 (6)	0.0163 (6)	0.0276 (7)	0.0000 (5)	-0.0046 (5)	-0.0104 (5)
C5	0.0141 (6)	0.0180 (6)	0.0202 (6)	-0.0027 (4)	-0.0052 (5)	-0.0060 (5)
C6	0.0115 (5)	0.0179 (6)	0.0217 (6)	0.0008 (4)	-0.0064 (5)	-0.0051 (5)
C7	0.0138 (6)	0.0132 (5)	0.0184 (6)	0.0005 (4)	-0.0049 (5)	-0.0044 (4)
C8	0.0157 (6)	0.0299 (7)	0.0362 (8)	-0.0023 (5)	-0.0087 (6)	-0.0159 (6)
C9	0.0121 (5)	0.0142 (5)	0.0136 (6)	-0.0012 (4)	-0.0049 (4)	-0.0029 (4)
C10	0.0126 (5)	0.0144 (5)	0.0129 (5)	0.0001 (4)	-0.0054 (4)	-0.0042 (4)
C11	0.0181 (6)	0.0221 (6)	0.0119 (6)	-0.0033 (5)	-0.0055 (5)	-0.0009 (5)
C12	0.0157 (6)	0.0222 (6)	0.0167 (6)	-0.0058 (5)	-0.0038 (5)	-0.0004 (5)
C13	0.0119 (5)	0.0178 (6)	0.0167 (6)	-0.0018 (4)	-0.0050 (5)	-0.0041 (5)
C14	0.0139 (5)	0.0160 (5)	0.0138 (6)	0.0001 (4)	-0.0060 (4)	-0.0050 (4)

Geometric parameters (Å, °)

Co1—O1	2.0864 (8)	C3—C4	1.3819 (17)
Co1—O1 ⁱ	2.0864 (8)	C3—H3	0.9300

Co1—O5	2.1254 (9)	C4—H4	0.9300
Co1—O5 ⁱ	2.1254 (9)	C5—C4	1.3932 (18)
Co1—N1	2.1276 (10)	C5—C8	1.4804 (18)
Co1—N1 ⁱ	2.1276 (10)	C6—C5	1.3884 (17)
O1—C1	1.2610 (14)	C6—C7	1.3907 (17)
O2—C1	1.2608 (15)	C6—H6	0.9300
O3—C8	1.2014 (18)	C7—H7	0.9300
O4—C14	1.2391 (15)	C8—H8	0.973 (18)
O5—H51	0.81 (2)	C9—H9	0.9300
O5—H52	0.86 (2)	C10—C9	1.3858 (17)
N1—C9	1.3415 (15)	C10—C11	1.3904 (17)
N1—C13	1.3433 (15)	C10—C14	1.5005 (16)
N2—C14	1.3267 (16)	C11—C12	1.3873 (18)
N2—H21	0.870 (19)	C11—H11	0.9300
N2—H22	0.861 (19)	C12—H12	0.9300
C1—C2	1.5090 (16)	C13—C12	1.3828 (18)
C2—C3	1.3990 (17)	C13—H13	0.9300
C2—C7	1.3903 (17)		
O1 ⁱ —Co1—O1	180.00 (2)	C3—C4—C5	119.70 (11)
O1—Co1—O5	87.96 (3)	C3—C4—H4	120.1
O1 ⁱ —Co1—O5	92.04 (3)	C5—C4—H4	120.1
O1—Co1—O5 ⁱ	92.04 (3)	C4—C5—C8	121.27 (12)
O1 ⁱ —Co1—O5 ⁱ	87.96 (3)	C6—C5—C4	120.33 (11)
O1—Co1—N1	89.61 (4)	C6—C5—C8	118.41 (12)
O1 ⁱ —Co1—N1	90.39 (4)	C5—C6—C7	120.04 (11)
O1—Co1—N1 ⁱ	90.39 (4)	C5—C6—H6	120.0
O1 ⁱ —Co1—N1 ⁱ	89.61 (4)	C7—C6—H6	120.0
O5 ⁱ —Co1—O5	180.0	C2—C7—C6	119.75 (11)
O5—Co1—N1	92.20 (4)	C2—C7—H7	120.1
O5 ⁱ —Co1—N1	87.80 (4)	C6—C7—H7	120.1
O5—Co1—N1 ⁱ	87.80 (4)	O3—C8—C5	124.84 (13)
O5 ⁱ —Co1—N1 ⁱ	92.20 (4)	O3—C8—H8	120.3 (10)
N1—Co1—N1 ⁱ	180.00 (6)	C5—C8—H8	114.8 (10)
C1—O1—Co1	127.04 (8)	N1—C9—C10	123.26 (11)
Co1—O5—H51	124.5 (13)	N1—C9—H9	118.4
Co1—O5—H52	98.6 (14)	C10—C9—H9	118.4
H52—O5—H51	104.8 (18)	C9—C10—C11	118.10 (11)
C9—N1—Co1	119.37 (8)	C9—C10—C14	117.60 (11)
C9—N1—C13	118.05 (11)	C11—C10—C14	124.27 (11)
C13—N1—Co1	122.58 (8)	C10—C11—H11	120.5
C14—N2—H21	123.1 (12)	C12—C11—C10	119.07 (12)
C14—N2—H22	117.7 (12)	C12—C11—H11	120.5
H21—N2—H22	118.5 (17)	C11—C12—H12	120.5
O1—C1—C2	117.52 (10)	C13—C12—C11	119.01 (12)
O2—C1—O1	125.58 (11)	C13—C12—H12	120.5
O2—C1—C2	116.84 (10)	N1—C13—C12	122.50 (11)
C3—C2—C1	120.06 (11)	N1—C13—H13	118.7

C7—C2—C1	119.83 (11)	C12—C13—H13	118.7
C7—C2—C3	119.96 (11)	O4—C14—N2	122.48 (11)
C2—C3—H3	119.9	O4—C14—C10	119.74 (11)
C4—C3—C2	120.18 (11)	N2—C14—C10	117.73 (11)
C4—C3—H3	119.9		
O5—Co1—O1—C1	-153.43 (10)	C1—C2—C3—C4	173.96 (12)
O5 ⁱ —Co1—O1—C1	26.57 (10)	C7—C2—C3—C4	-1.47 (19)
N1—Co1—O1—C1	114.35 (10)	C1—C2—C7—C6	-173.32 (11)
N1 ⁱ —Co1—O1—C1	-65.65 (10)	C3—C2—C7—C6	2.12 (19)
O1—Co1—N1—C9	-143.16 (9)	C2—C3—C4—C5	-0.5 (2)
O1 ⁱ —Co1—N1—C9	36.84 (9)	C6—C5—C4—C3	1.9 (2)
O1—Co1—N1—C13	37.41 (9)	C8—C5—C4—C3	-178.06 (13)
O1 ⁱ —Co1—N1—C13	-142.59 (9)	C4—C5—C8—O3	4.7 (3)
O5—Co1—N1—C9	128.90 (9)	C6—C5—C8—O3	-175.19 (16)
O5 ⁱ —Co1—N1—C9	-51.10 (9)	C7—C6—C5—C4	-1.2 (2)
O5—Co1—N1—C13	-50.53 (10)	C7—C6—C5—C8	178.71 (13)
O5 ⁱ —Co1—N1—C13	129.47 (10)	C5—C6—C7—C2	-0.78 (19)
Co1—O1—C1—O2	-20.75 (17)	C11—C10—C9—N1	-0.79 (18)
Co1—O1—C1—C2	156.34 (8)	C14—C10—C9—N1	177.53 (11)
Co1—N1—C9—C10	-178.76 (9)	C9—C10—C11—C12	0.23 (18)
C13—N1—C9—C10	0.70 (18)	C14—C10—C11—C12	-177.97 (12)
Co1—N1—C13—C12	179.38 (9)	C9—C10—C14—O4	-1.39 (17)
C9—N1—C13—C12	-0.06 (18)	C9—C10—C14—N2	-179.18 (11)
O1—C1—C2—C3	161.25 (11)	C11—C10—C14—O4	176.81 (12)
O1—C1—C2—C7	-23.31 (17)	C11—C10—C14—N2	-0.97 (18)
O2—C1—C2—C3	-21.40 (17)	C10—C11—C12—C13	0.35 (19)
O2—C1—C2—C7	154.03 (12)	N1—C13—C12—C11	-0.5 (2)

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

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

Cg is the centroid of the pyridine ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H21 \cdots O2 ⁱⁱ	0.87 (2)	2.078 (19)	2.8834 (15)	153 (2)
N2—H22 \cdots O4 ⁱⁱⁱ	0.86 (2)	2.04 (2)	2.8908 (16)	167 (2)
O5—H51 \cdots O4 ^{iv}	0.81 (2)	2.08 (2)	2.8583 (13)	162.3 (19)
O5—H52 \cdots O2 ⁱ	0.87 (2)	1.83 (2)	2.6774 (14)	164 (2)
C6—H6 \cdots O2 ^{iv}	0.93	2.39	3.3123 (17)	172
C13—H13 \cdots O3 ^v	0.93	2.47	3.3120 (18)	150
C4—H4 \cdots Cg ^{vi}	0.93	2.72	3.6338 (14)	167

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, y, z-1$; (iii) $-x-1, -y, -z-1$; (iv) $x+1, y, z$; (v) $-x+1, -y+1, -z$; (vi) $-x, -y+1, -z+2$.