

## Diaquabis(2-chlorobenzoato- $\kappa$ O)bis-(nicotinamide- $\kappa$ N<sup>1</sup>)cobalt(II)

Öznur Dincel,<sup>a</sup> Barış Tercan,<sup>a</sup> Füreyâ Elif Öztürkkan,<sup>b</sup> Hacali Necefoğlu<sup>b</sup> and Tuncer Hökelek<sup>c\*</sup>

<sup>a</sup>Department of Physics, Karabük University, 78050 Karabük, Turkey, <sup>b</sup>Department of Chemistry, Kafkas University, 36100 Kars, Turkey, and <sup>c</sup>Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey

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

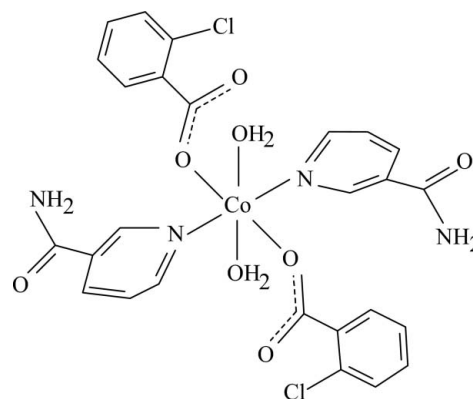
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.088;  $wR$  factor = 0.237; data-to-parameter ratio = 16.3.

In the title complex,  $[\text{Co}(\text{C}_7\text{H}_4\text{ClO}_2)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$ , the  $\text{Co}^{\text{II}}$  cation is located on an inversion center and is coordinated by two 2-chlorobenzoate anions, two nicotinamide (NA) ligands and two water molecules. The four O atoms in the equatorial plane around the  $\text{Co}^{\text{II}}$  cation form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two pyridine N atoms of the NA ligands in the axial positions. The dihedral angle between the carboxylate group and the adjacent benzene ring is  $29.7(4)^\circ$ , while the pyridine and benzene rings are oriented at a dihedral angle of  $83.17(15)^\circ$ . Intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonding occurs between the carboxylate group and coordinating water molecule. In the crystal, intermolecular  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{O}-\text{H}\cdots\text{O}$  and weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into a three-dimensional network.

### Related literature

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



### Experimental

#### Crystal data

$[\text{Co}(\text{C}_7\text{H}_4\text{ClO}_2)_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$   
 $M_r = 650.32$   
 Monoclinic,  $P2_1/n$   
 $a = 7.8679(2)$  Å  
 $b = 17.9522(3)$  Å  
 $c = 9.8492(2)$  Å

$\beta = 106.637(3)^\circ$   
 $V = 1332.92(5)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.90$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.39 \times 0.33 \times 0.23$  mm

#### Data collection

Bruker Kappa APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\text{min}} = 0.708$ ,  $T_{\text{max}} = 0.811$

10778 measured reflections  
 3285 independent reflections  
 2366 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.061$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.088$   
 $wR(F^2) = 0.237$   
 $S = 1.23$   
 3285 reflections  
 202 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.42$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.61$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Co1—N1	2.129 (4)	Co1—O4	2.153 (4)
Co1—O2	2.102 (4)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H21 <sup>i</sup> ···O1 <sup>i</sup>	0.82 (10)	2.11 (9)	2.861 (6)	152 (9)
N2—H22 <sup>ii</sup> ···O3 <sup>iii</sup>	0.90 (7)	2.20 (6)	2.932 (7)	138 (5)
O4—H41 <sup>i</sup> ···O3 <sup>iii</sup>	0.78 (9)	2.20 (10)	2.890 (6)	147 (10)
O4—H42 <sup>i</sup> ···O1	0.96 (9)	1.72 (9)	2.628 (7)	155 (8)
C6—H6 <sup>i</sup> ···O1 <sup>iv</sup>	0.93	2.55	3.468 (8)	170
Cl10—H10 <sup>i</sup> ···O1 <sup>i</sup>	0.93	2.60	3.476 (7)	158

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

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, 2012) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 2012) and PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5678).

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## supporting information

*Acta Cryst.* (2013). E69, m173–m174 [doi:10.1107/S1600536813004984]

**Diaquabis(2-chlorobenzoato- $\kappa$ O)bis(nicotinamide- $\kappa$ N<sup>1</sup>)cobalt(II)****Öznur Dincel, Barış Tercan, Füreyâ Elif Öztürkkan, Hacali Necefoğlu and Tuncer Hökelek****S1. Comment**

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

The title compound, (I), is a mononuclear complex, where the Co<sup>II</sup> ion is located on a crystallographic inversion center. The asymmetric unit contains one 2-chlorobenzoate (CB) anion, one nicotinamide (NA) ligand and one coordinated water molecule, all ligands are monodentate (Fig. 1). The crystal structures of similar complexes of Cu<sup>II</sup>, Co<sup>II</sup>, Ni<sup>II</sup>, Mn<sup>II</sup> and Zn<sup>II</sup> ions, [Cu(C<sub>7</sub>H<sub>5</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O)<sub>2</sub>] (Hökelek *et al.*, 1996), [Cu(C<sub>7</sub>H<sub>4</sub>BrO<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] (Necefoğlu *et al.*, 2011a), [Co(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(C<sub>7</sub>H<sub>4</sub>NO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] (Hökelek & Necefoğlu, 1998), [Co(C<sub>9</sub>H<sub>9</sub>O<sub>2</sub>)<sub>2</sub>(C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] (Necefoğlu *et al.*, 2011b), [Ni(C<sub>7</sub>H<sub>4</sub>ClO<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] (Hökelek *et al.*, 2009a), [Mn(C<sub>9</sub>H<sub>10</sub>NO<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>].2H<sub>2</sub>O (Hökelek & Necefoğlu, 2007) and [Zn(C<sub>7</sub>H<sub>4</sub>BrO<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] (Hökelek *et al.*, 2009b) have also been reported. In the copper(II) complex mentioned above the two benzoate ions coordinate to the Cu<sup>II</sup> 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 (O2, O2', O4 and O4') in the equatorial plane around the Co<sup>II</sup> 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 (Fig. 1).

The near equalities of the C1—O1 [1.254 (7) Å] and C1—O2 [1.273 (7) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds. The Co—O bond lengths are 2.102 (4) Å (for benzoate oxygens) and 2.153 (4) Å (for water oxygens), and the Co—N bond length is 2.129 (4) Å, close to standard values (Allen *et al.*, 1987). The Co atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by -0.6474 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring A (C2—C7) is 29.65 (41)°, while that between rings A and B (N1/C8—C12) is 83.17 (15)°. Intramolecular O—H...O hydrogen bonding occurs between the carboxylate group and coordinated water molecule (Table 1, Fig. 1).

In the crystal structure, 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.

**S2. Experimental**

The title compound was prepared by the reaction of CoSO<sub>4</sub>·7H<sub>2</sub>O (1.40 g, 5 mmol) in H<sub>2</sub>O (40 ml) and nicotinamide (1.78 g, 10 mmol) in H<sub>2</sub>O (20 ml) with sodium 2-chlorobenzoate (2.23 g, 10 mmol) in H<sub>2</sub>O (50 ml). The mixture was filtered and set aside to crystallize at ambient temperature for two weeks, giving pink single crystals (yield; 3.065 g, 72%).

## S3. Refinement

Atoms H21, H22 (for NH<sub>2</sub>) and H41, H42 (for H<sub>2</sub>O) were located in a difference Fourier map and refined isotropically. 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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The highest residual electron density was found 1.17 Å from Co1 and the deepest hole 0.80 Å from Co1.

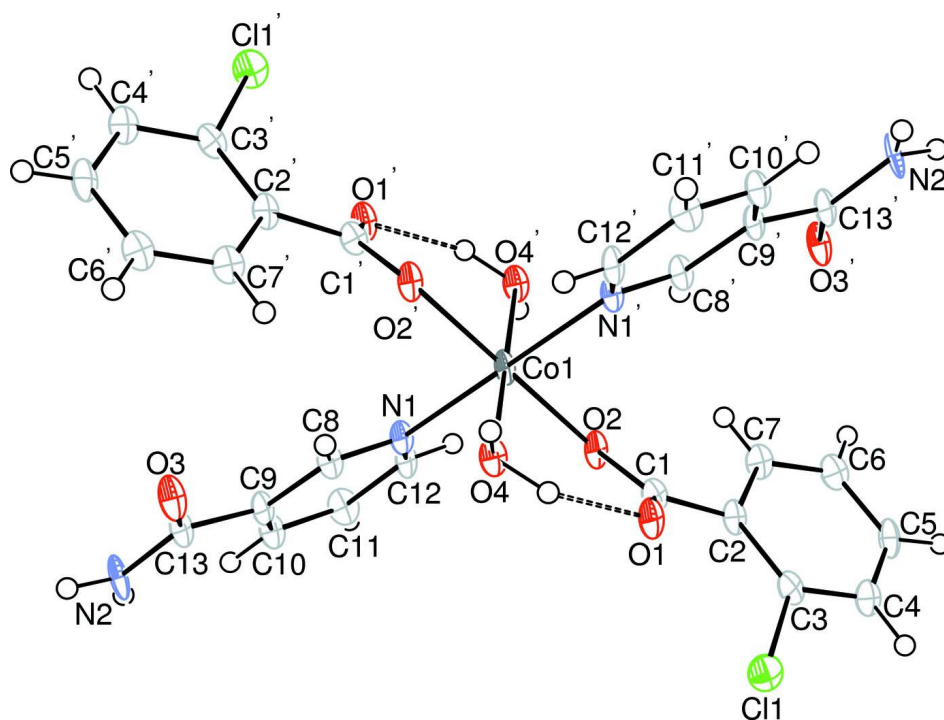


Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator: (') 1-*x*, -*y*, -*z*.

Diaquabis(2-chlorobenzoato- $\kappa$ O)bis(nicotinamide- $\kappa$ N<sup>1</sup>)cobalt(II)

## Crystal data

[Co(C<sub>7</sub>H<sub>4</sub>ClO<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 650.32$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 7.8679$  (2) Å

$b = 17.9522$  (3) Å

$c = 9.8492$  (2) Å

$\beta = 106.637$  (3)°

$V = 1332.92$  (5) Å<sup>3</sup>

$Z = 2$

$F(000) = 666$

$D_x = 1.620$  Mg m<sup>-3</sup>

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

Cell parameters from 4735 reflections

$\theta = 2.4$ – $27.9$ °

$\mu = 0.90$  mm<sup>-1</sup>

$T = 100$  K

Block, pink

$0.39 \times 0.33 \times 0.23$  mm

## Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\text{min}} = 0.708$ ,  $T_{\text{max}} = 0.811$

10778 measured reflections

3285 independent reflections

2366 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.061$   
 $\theta_{\text{max}} = 28.3^\circ$ ,  $\theta_{\text{min}} = 2.3^\circ$

$h = -6 \rightarrow 10$   
 $k = -23 \rightarrow 18$   
 $l = -13 \rightarrow 12$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.088$   
 $wR(F^2) = 0.237$   
 $S = 1.23$   
 3285 reflections  
 202 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0784P)^2 + 7.9389P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 1.42 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.61 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.0000	0.0169 (3)
Cl1	-0.0922 (2)	0.28811 (9)	-0.32577 (17)	0.0282 (4)
O1	-0.1130 (5)	0.1367 (2)	-0.2254 (4)	0.0223 (9)
O2	0.1155 (5)	0.0988 (2)	-0.0461 (4)	0.0192 (8)
O3	-0.4515 (5)	0.0095 (3)	0.3249 (4)	0.0250 (10)
O4	-0.2634 (6)	0.0436 (3)	-0.0890 (4)	0.0211 (9)
H41	-0.329 (12)	0.014 (5)	-0.133 (10)	0.04 (3)*
H42	-0.241 (11)	0.084 (5)	-0.146 (9)	0.05 (2)*
N1	-0.0041 (6)	0.0446 (3)	0.1993 (5)	0.0175 (10)
N2	-0.3567 (7)	0.0816 (3)	0.5201 (5)	0.0244 (12)
H21	-0.282 (12)	0.108 (5)	0.573 (10)	0.05 (3)*
H22	-0.457 (8)	0.071 (3)	0.543 (7)	0.013 (15)*
C1	0.0477 (7)	0.1383 (3)	-0.1558 (6)	0.0180 (11)
C2	0.1707 (8)	0.1857 (3)	-0.2106 (6)	0.0188 (11)
C3	0.1181 (8)	0.2488 (3)	-0.2961 (6)	0.0196 (11)
C4	0.2310 (8)	0.2848 (4)	-0.3596 (6)	0.0214 (12)
H4	0.1919	0.3263	-0.4166	0.026*
C5	0.4023 (8)	0.2589 (4)	-0.3380 (6)	0.0236 (12)
H5	0.4774	0.2818	-0.3830	0.028*
C6	0.4619 (8)	0.1984 (4)	-0.2485 (6)	0.0233 (12)
H6	0.5784	0.1821	-0.2303	0.028*

C7	0.3468 (8)	0.1629 (4)	-0.1870 (6)	0.0207 (12)
H7	0.3879	0.1224	-0.1278	0.025*
C8	-0.1512 (7)	0.0371 (3)	0.2405 (5)	0.0179 (11)
H8	-0.2469	0.0113	0.1819	0.021*
C9	-0.1672 (7)	0.0661 (3)	0.3663 (5)	0.0173 (11)
C10	-0.0260 (8)	0.1057 (3)	0.4526 (6)	0.0211 (12)
H10	-0.0339	0.1267	0.5369	0.025*
C11	0.1259 (8)	0.1134 (4)	0.4115 (6)	0.0227 (12)
H11	0.2225	0.1395	0.4680	0.027*
C12	0.1337 (7)	0.0817 (3)	0.2846 (5)	0.0189 (11)
H12	0.2375	0.0863	0.2581	0.023*
C13	-0.3372 (7)	0.0508 (3)	0.4019 (6)	0.0188 (12)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0160 (5)	0.0304 (6)	0.0024 (4)	-0.0006 (4)	0.000	-0.0003 (4)
C11	0.0217 (7)	0.0377 (9)	0.0220 (8)	0.0073 (6)	0.0009 (6)	0.0057 (6)
O1	0.019 (2)	0.039 (3)	0.0062 (18)	-0.0013 (17)	-0.0009 (15)	0.0015 (17)
O2	0.0159 (19)	0.035 (2)	0.0026 (17)	-0.0021 (16)	-0.0033 (15)	0.0011 (15)
O3	0.019 (2)	0.047 (3)	0.0072 (18)	-0.0064 (18)	0.0008 (15)	-0.0044 (18)
O4	0.020 (2)	0.034 (3)	0.0059 (19)	-0.0020 (18)	-0.0014 (16)	-0.0009 (18)
N1	0.018 (2)	0.029 (3)	0.004 (2)	-0.0013 (19)	-0.0005 (17)	-0.0005 (18)
N2	0.019 (3)	0.049 (4)	0.007 (2)	-0.007 (2)	0.007 (2)	-0.006 (2)
C1	0.017 (2)	0.027 (3)	0.007 (2)	-0.001 (2)	-0.001 (2)	-0.003 (2)
C2	0.020 (3)	0.029 (3)	0.004 (2)	-0.004 (2)	-0.001 (2)	-0.003 (2)
C3	0.018 (3)	0.031 (3)	0.007 (2)	0.001 (2)	-0.001 (2)	-0.004 (2)
C4	0.021 (3)	0.032 (3)	0.007 (3)	-0.003 (2)	-0.002 (2)	-0.001 (2)
C5	0.024 (3)	0.038 (3)	0.008 (3)	-0.007 (3)	0.004 (2)	-0.002 (2)
C6	0.019 (3)	0.034 (3)	0.015 (3)	-0.002 (2)	0.001 (2)	-0.004 (2)
C7	0.018 (3)	0.031 (3)	0.008 (2)	-0.002 (2)	-0.004 (2)	-0.002 (2)
C8	0.016 (3)	0.030 (3)	0.004 (2)	-0.002 (2)	-0.002 (2)	-0.002 (2)
C9	0.014 (2)	0.030 (3)	0.006 (2)	0.002 (2)	0.001 (2)	0.002 (2)
C10	0.023 (3)	0.032 (3)	0.006 (2)	-0.003 (2)	0.001 (2)	-0.004 (2)
C11	0.018 (3)	0.036 (3)	0.008 (3)	-0.003 (2)	-0.006 (2)	-0.005 (2)
C12	0.015 (3)	0.035 (3)	0.005 (2)	0.000 (2)	0.000 (2)	0.002 (2)
C13	0.013 (2)	0.036 (3)	0.006 (2)	0.000 (2)	0.000 (2)	0.001 (2)

*Geometric parameters (Å, °)*

Co1—N1	2.129 (4)	C2—C7	1.399 (8)
Co1—N1 <sup>i</sup>	2.129 (4)	C3—C4	1.384 (8)
Co1—O2	2.102 (4)	C4—C5	1.383 (8)
Co1—O2 <sup>i</sup>	2.102 (4)	C4—H4	0.9300
Co1—O4	2.153 (4)	C5—H5	0.9300
Co1—O4 <sup>i</sup>	2.153 (4)	C6—C5	1.392 (9)
C11—C3	1.744 (6)	C6—H6	0.9300
O1—C1	1.254 (7)	C7—C6	1.381 (8)

O2—C1	1.273 (7)	C7—H7	0.9300
O3—C13	1.243 (7)	C8—H8	0.9300
O4—H41	0.78 (9)	C9—C8	1.382 (7)
O4—H42	0.96 (9)	C9—C10	1.386 (8)
N1—C8	1.339 (7)	C9—C13	1.502 (7)
N1—C12	1.343 (7)	C10—C11	1.374 (8)
N2—C13	1.337 (7)	C10—H10	0.9300
N2—H21	0.81 (9)	C11—H11	0.9300
N2—H22	0.90 (6)	C12—C11	1.390 (8)
C1—C2	1.501 (8)	C12—H12	0.9300
C2—C3	1.402 (8)		
O2—Co1—O2 <sup>i</sup>	180.0 (2)	C4—C3—C2	122.1 (5)
O2—Co1—O4	91.75 (17)	C4—C3—C11	115.9 (5)
O2 <sup>i</sup> —Co1—O4	88.25 (17)	C3—C4—H4	120.1
O2—Co1—O4 <sup>i</sup>	88.25 (17)	C5—C4—C3	119.8 (6)
O2 <sup>i</sup> —Co1—O4 <sup>i</sup>	91.75 (17)	C5—C4—H4	120.1
O2—Co1—N1	90.19 (16)	C4—C5—C6	119.7 (5)
O2 <sup>i</sup> —Co1—N1	89.81 (16)	C4—C5—H5	120.1
O2—Co1—N1 <sup>i</sup>	89.81 (16)	C6—C5—H5	120.1
O2 <sup>i</sup> —Co1—N1 <sup>i</sup>	90.19 (16)	C5—C6—H6	120.2
O4—Co1—O4 <sup>i</sup>	180.0 (2)	C7—C6—C5	119.6 (6)
N1—Co1—O4	88.39 (17)	C7—C6—H6	120.2
N1 <sup>i</sup> —Co1—N1	180.0 (3)	C2—C7—H7	118.8
N1 <sup>i</sup> —Co1—O4	91.61 (17)	C6—C7—C2	122.3 (6)
N1—Co1—O4 <sup>i</sup>	91.61 (17)	C6—C7—H7	118.8
N1 <sup>i</sup> —Co1—O4 <sup>i</sup>	88.39 (17)	N1—C8—C9	122.8 (5)
C1—O2—Co1	123.4 (4)	N1—C8—H8	118.6
Co1—O4—H41	113 (6)	C9—C8—H8	118.6
Co1—O4—H42	101 (5)	C8—C9—C10	118.7 (5)
H41—O4—H42	113 (8)	C8—C9—C13	117.1 (5)
C8—N1—Co1	119.0 (4)	C10—C9—C13	124.1 (5)
C8—N1—C12	118.3 (5)	C9—C10—H10	120.6
C12—N1—Co1	122.8 (4)	C11—C10—C9	118.9 (5)
C13—N2—H21	124 (6)	C11—C10—H10	120.6
C13—N2—H22	117 (4)	C10—C11—C12	119.3 (5)
H22—N2—H21	119 (7)	C10—C11—H11	120.4
O1—C1—O2	124.2 (5)	C12—C11—H11	120.4
O1—C1—C2	118.0 (5)	N1—C12—C11	122.0 (5)
O2—C1—C2	117.6 (5)	N1—C12—H12	119.0
C3—C2—C1	124.4 (5)	C11—C12—H12	119.0
C7—C2—C1	119.0 (5)	O3—C13—N2	122.3 (5)
C7—C2—C3	116.4 (5)	O3—C13—C9	120.2 (5)
C2—C3—C11	122.0 (4)	N2—C13—C9	117.4 (5)
O4—Co1—O2—C1	-34.9 (4)	C1—C2—C3—C11	10.4 (8)
O4 <sup>i</sup> —Co1—O2—C1	145.1 (4)	C1—C2—C3—C4	-171.1 (5)
N1—Co1—O2—C1	-123.3 (4)	C7—C2—C3—C11	-175.5 (4)

N1 <sup>i</sup> —Co1—O2—C1	56.7 (4)	C7—C2—C3—C4	3.0 (8)
O2—Co1—N1—C8	134.5 (4)	C1—C2—C7—C6	171.9 (5)
O2 <sup>i</sup> —Co1—N1—C8	-45.5 (4)	C3—C2—C7—C6	-2.5 (8)
O2—Co1—N1—C12	-43.9 (4)	C11—C3—C4—C5	177.9 (4)
O2 <sup>i</sup> —Co1—N1—C12	136.1 (4)	C2—C3—C4—C5	-0.7 (9)
O4—Co1—N1—C8	42.8 (4)	C3—C4—C5—C6	-2.3 (9)
O4 <sup>i</sup> —Co1—N1—C8	-137.2 (4)	C7—C6—C5—C4	2.7 (9)
O4—Co1—N1—C12	-135.6 (5)	C2—C7—C6—C5	-0.3 (9)
O4 <sup>i</sup> —Co1—N1—C12	44.4 (5)	C10—C9—C8—N1	1.1 (9)
Co1—O2—C1—O1	21.7 (8)	C13—C9—C8—N1	-177.6 (5)
Co1—O2—C1—C2	-154.0 (4)	C8—C9—C10—C11	-1.3 (9)
Co1—N1—C8—C9	-178.2 (4)	C13—C9—C10—C11	177.2 (6)
C12—N1—C8—C9	0.3 (9)	C8—C9—C13—O3	4.8 (8)
Co1—N1—C12—C11	177.0 (4)	C8—C9—C13—N2	-176.9 (6)
C8—N1—C12—C11	-1.4 (8)	C10—C9—C13—O3	-173.8 (6)
O1—C1—C2—C3	26.3 (8)	C10—C9—C13—N2	4.5 (9)
O1—C1—C2—C7	-147.6 (5)	C9—C10—C11—C12	0.3 (9)
O2—C1—C2—C3	-157.8 (5)	N1—C12—C11—C10	1.1 (9)
O2—C1—C2—C7	28.3 (8)		

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

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H21 $\cdots$ O1 <sup>ii</sup>	0.82 (10)	2.11 (9)	2.861 (6)	152 (9)
N2—H22 $\cdots$ O3 <sup>iii</sup>	0.90 (7)	2.20 (6)	2.932 (7)	138 (5)
O4—H41 $\cdots$ O3 <sup>iv</sup>	0.78 (9)	2.20 (10)	2.890 (6)	147 (10)
O4—H42 $\cdots$ O1	0.96 (9)	1.72 (9)	2.628 (7)	155 (8)
C6—H6 $\cdots$ O1 <sup>v</sup>	0.93	2.55	3.468 (8)	170
C10—H10 $\cdots$ O1 <sup>ii</sup>	0.93	2.60	3.476 (7)	158

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