Diaquabis(2-iodobenzoato-κO)bis-(nicotinamide-κN^1)cobalt(II)

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In the title complex, $[Co(C_7H_4IO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, the Co^{II} cation is located on an inversion center and is coordinated by two monodentate 2-iodobenzoate (IB) 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 22.3 (3)°, while the pyridine ring and the benzene ring are oriented at a dihedral angle of 84.59 (13)°. Intramolecular O—H⋯O hydrogen bonding occurs between the carboxylate group and coordinated water molecule. In the crystal, N—H⋯O, O—H⋯O and weak C—H⋯O hydrogen bonds link the molecules into a three-dimensional supramolecular network.

Related literature

For niacin, see: Krishnamachari (1974). For 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).
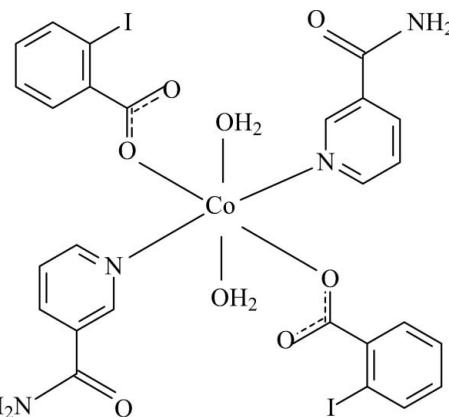
Experimental

Crystal data

$[Co(C_7H_4IO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$	V = 1444.07 (7) Å^3
M_r = 833.22	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 7.9475 (2) Å	μ = 2.79 mm^{-1}
b = 19.7551 (4) Å	T = 100 K
c = 9.7070 (3) Å	$0.35 \times 0.22 \times 0.17$ mm
β = 108.642 (3)°	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	12419 measured reflections
	3618 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	3378 reflections with $I > 2\sigma(I)$
T_{min} = 0.484, T_{max} = 0.623	R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.110	
S = 1.16	
3618 reflections	$\Delta\rho_{max}$ = 2.60 e Å^{-3}
203 parameters	$\Delta\rho_{min}$ = −2.03 e Å^{-3}
6 restraints	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H21⋯O1^i	0.86 (6)	2.02 (6)	2.837 (6)	158 (5)
N2—H22⋯O3^{ii}	0.86 (6)	2.21 (7)	2.984 (7)	151 (7)
O4—H41⋯O3^{iii}	0.86 (5)	2.00 (5)	2.827 (5)	162 (5)
O4—H42⋯O1	0.86 (5)	1.80 (6)	2.631 (5)	161 (7)
C10—H10⋯O1^i	0.93	2.51	3.400 (6)	160

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

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, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

metal-organic compounds

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supplementary materials

Diaquabis(2-iodobenzoato-*κO*)bis(nicotinamide-*κN*¹)cobalt(II)

Ömür Aydın, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek

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 (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title mononuclear Co^{II}complex, (Fig. 1), contains one-half molecule. It consists of two nicotinamide (NA), two 2-iodobenzoate (IB) ligands and two coordinated water molecules, all ligands coordinating in a monodentate manner. The crystal structures of similar complexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions, [Cu(C$_7$H$_5$O$_2$)$_2$(C$_{10}$H$_{14}$N$_2$O)$_2$] (Hökelek *et al.*, 1996), [Cu(C$_7$H$_4$BrO$_2$)$_2$(C$_6$H$_6$N$_2$O)$_2$(H$_2$O)$_2$] (Necefoğlu *et al.*, 2011*a*), [Co(C$_6$H$_6$N$_2$O)$_2$(C$_7$H$_4$NO$_4$)$_2$(H$_2$O)$_2$] (Hökelek & Necefoğ˘lu, 1998), [Co(C$_9$H$_9$O$_2$)$_2$(C$_{10}$H$_{14}$N$_2$O)$_2$(H$_2$O)$_2$] (Necefoğlu *et al.*, 2011*b*), [Ni(C$_7$H$_4$ClO$_2$)$_2$(C$_6$H$_6$N$_2$O)$_2$(H$_2$O)$_2$] (Hökelek *et al.*, 2009*a*), [Mn(C$_9$H$_{10}$NO$_2$)$_2$(H$_2$O)$_4$].2H$_2$O (Hökelek & Necefoğlu, 2007) and [Zn(C$_7$H$_4$BrO$_2$)$_2$(C$_6$H$_6$N$_2$O)$_2$(H$_2$O)$_2$] (Hökelek *et al.*, 2009*b*) 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 (O2, O2′, O4 and O4′) 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 [1.253 (6) Å] and C1—O2 [1.263 (6) Å] bonds in the carboxylate group indicate delocalized bonding arrangement, rather than localized single and double bonds. The Co—O bond lengths are 2.077 (3) Å (for benzoate oxygens) and 2.135 (4) Å (for water oxygens), and the Co—N bond length is 2.134 (4) 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 0.5765 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring A (C2—C7) is 22.33 (31)°. The benzene A (C2 —C7) and the pyridine B (N1/C8—C12) rings are oriented at a dihedral angle of A/B = 84.59 (13)°.

In the crystal, intermolecular N—H···O, O—H···O and C—H···O hydrogen bonds (Table 1) link the molecules into a three-dimensional network.

Experimental

The title compound was prepared by the reaction of CoSO$_4$.7H$_2$O (1.406 g, 5 mmol) in H$_2$O (20 ml) and NA (1.220 g, 10 mmol) in H$_2$O (20 ml) with sodium 2-iodobenzoate (2.700 g, 10 mmol) in H$_2$O (100 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving orange single crystals.

Refinement

Atoms H21 and H22 (for NH$_2$) and H41 and H42 (for H$_2$O) were located in a difference Fourier map and were refined by applying restraints. 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 $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron density was found 0.87 Å from I1 and the deepest hole 1.30 Å from C5.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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).
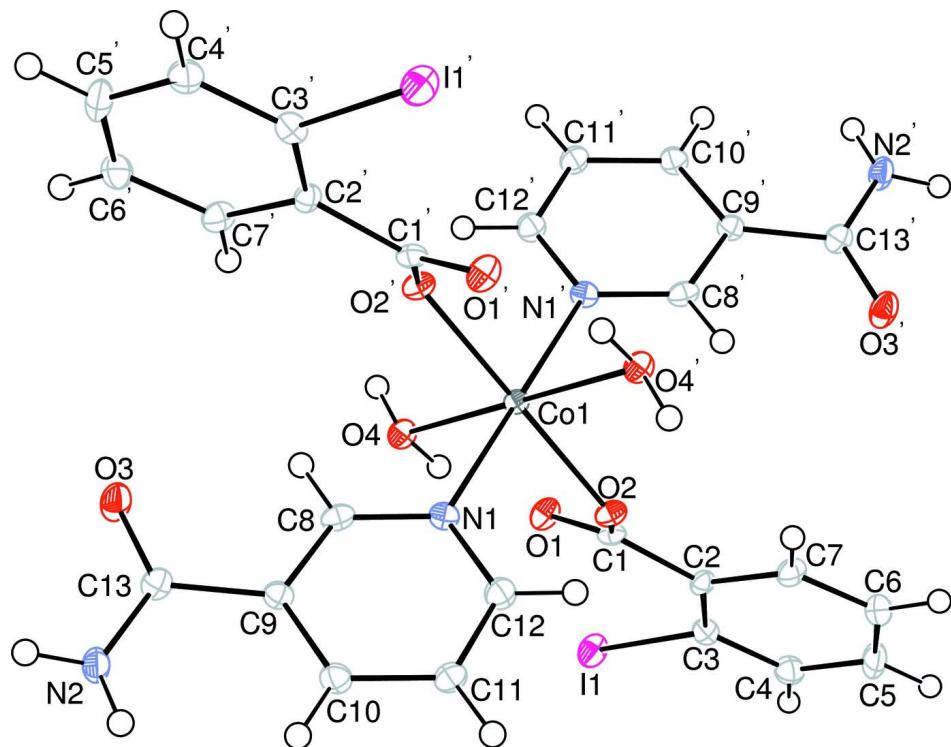
Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (') -x, 1-y, -z].

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Crystal data

[Co(C₇H₄IO₂)₂(C₆H₆N₂O)₂(H₂O)₂]	$F(000) = 810$
$M_r = 833.22$	$D_x = 1.916$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 8593 reflections
$a = 7.9475$ (2) Å	$\theta = 2.4–28.5°$
$b = 19.7551$ (4) Å	$\mu = 2.79$ mm⁻¹
$c = 9.7070$ (3) Å	$T = 100$ K
$\beta = 108.642$ (3)°	Block, pink
$V = 1444.07$ (7) Å³	$0.35 \times 0.22 \times 0.17$ mm
$Z = 2$	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	12419 measured reflections
Radiation source: fine-focus sealed tube	3618 independent reflections
Graphite monochromator	3378 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.030$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$\theta_{max} = 28.5°$, $\theta_{min} = 2.1°$
$T_{min} = 0.484$, $T_{max} = 0.623$	$h = -10\rightarrow9$
	$k = -23\rightarrow26$
	$l = -12\rightarrow13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.110$	
$S = 1.16$	H atoms treated by a mixture of independent and constrained refinement
3618 reflections	
203 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2 + 14.519P]$
6 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 2.60$ e Å^{-3}
	$\Delta\rho_{min} = -2.03$ e Å^{-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 $F^2 > 2sigma(F^2)$ 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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
I1	0.12711 (5)	0.234042 (17)	0.36675 (4)	0.01979 (11)
Co1	0.0000	0.5000	0.0000	0.00988 (19)
O1	0.1064 (5)	0.37344 (19)	0.2233 (4)	0.0159 (7)
O2	−0.1200 (5)	0.41184 (18)	0.0387 (4)	0.0133 (7)
O3	0.4451 (5)	0.4942 (2)	−0.3249 (4)	0.0209 (8)
O4	0.2604 (5)	0.45921 (18)	0.0942 (4)	0.0143 (7)
H41	0.340 (7)	0.482 (3)	0.158 (5)	0.03 (2)*
H42	0.232 (9)	0.426 (2)	0.140 (6)	0.023 (17)*
N1	0.0033 (6)	0.4599 (2)	−0.2032 (4)	0.0123 (8)
N2	0.3548 (6)	0.4252 (3)	−0.5189 (5)	0.0189 (9)
H21	0.277 (7)	0.401 (3)	−0.582 (6)	0.022 (17)*
H22	0.443 (7)	0.439 (4)	−0.544 (8)	0.03 (2)*
C1	−0.0541 (7)	0.3739 (2)	0.1473 (5)	0.0123 (9)
C2	−0.1818 (6)	0.3282 (2)	0.1896 (5)	0.0120 (9)
C3	−0.1334 (7)	0.2707 (3)	0.2769 (5)	0.0137 (9)
C4	−0.2597 (7)	0.2321 (3)	0.3134 (6)	0.0179 (10)

H4	−0.2259	0.1933	0.3696	0.022*
C5	−0.4357 (8)	0.2521 (3)	0.2652 (6)	0.0224 (11)
H5	−0.5203	0.2264	0.2893	0.027*
C6	−0.4873 (7)	0.3098 (3)	0.1819 (6)	0.0196 (10)
H6	−0.6053	0.3237	0.1519	0.024*
C7	−0.3609 (7)	0.3466 (3)	0.1436 (5)	0.0154 (10)
H7	−0.3963	0.3848	0.0855	0.019*
C8	0.1496 (7)	0.4667 (2)	−0.2414 (5)	0.0133 (9)
H8	0.2449	0.4905	−0.1795	0.016*
C9	0.1669 (7)	0.4400 (2)	−0.3686 (5)	0.0125 (9)
C10	0.0245 (7)	0.4041 (3)	−0.4594 (5)	0.0149 (9)
H10	0.0312	0.3854	−0.5454	0.018*
C11	−0.1281 (7)	0.3965 (3)	−0.4207 (5)	0.0164 (10)
H11	−0.2246	0.3722	−0.4797	0.020*
C12	−0.1345 (7)	0.4255 (3)	−0.2930 (5)	0.0157 (10)
H12	−0.2378	0.4211	−0.2682	0.019*
C13	0.3344 (7)	0.4547 (3)	−0.4023 (5)	0.0143 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01340 (17)	0.01704 (18)	0.02576 (18)	0.00204 (12)	0.00180 (13)	0.00652 (13)
Co1	0.0102 (4)	0.0108 (4)	0.0076 (4)	−0.0005 (3)	0.0014 (3)	−0.0001 (3)
O1	0.0127 (17)	0.0198 (18)	0.0117 (15)	−0.0025 (14)	−0.0011 (13)	0.0023 (13)
O2	0.0149 (17)	0.0130 (17)	0.0096 (15)	−0.0024 (13)	0.0005 (13)	−0.0001 (12)
O3	0.0160 (19)	0.032 (2)	0.0151 (17)	−0.0088 (16)	0.0054 (15)	−0.0074 (15)
O4	0.0125 (17)	0.0159 (18)	0.0128 (15)	−0.0008 (13)	0.0016 (13)	0.0008 (13)
N1	0.014 (2)	0.013 (2)	0.0095 (17)	0.0006 (15)	0.0024 (15)	0.0000 (14)
N2	0.015 (2)	0.028 (3)	0.016 (2)	−0.0072 (18)	0.0081 (18)	−0.0081 (18)
C1	0.015 (2)	0.010 (2)	0.010 (2)	−0.0014 (18)	0.0032 (18)	−0.0025 (16)
C2	0.011 (2)	0.014 (2)	0.010 (2)	−0.0026 (17)	0.0020 (17)	−0.0017 (16)
C3	0.013 (2)	0.016 (2)	0.010 (2)	0.0013 (18)	0.0017 (18)	−0.0011 (17)
C4	0.019 (3)	0.015 (2)	0.020 (2)	0.001 (2)	0.007 (2)	0.0013 (19)
C5	0.016 (3)	0.026 (3)	0.029 (3)	−0.004 (2)	0.012 (2)	0.001 (2)
C6	0.014 (2)	0.020 (3)	0.025 (3)	0.000 (2)	0.007 (2)	−0.003 (2)
C7	0.012 (2)	0.015 (2)	0.016 (2)	−0.0004 (18)	−0.0005 (19)	0.0002 (18)
C8	0.014 (2)	0.011 (2)	0.011 (2)	−0.0011 (18)	−0.0003 (18)	0.0004 (16)
C9	0.013 (2)	0.013 (2)	0.010 (2)	0.0000 (18)	0.0023 (18)	−0.0010 (17)
C10	0.014 (2)	0.018 (2)	0.012 (2)	−0.0004 (19)	0.0029 (18)	−0.0030 (18)
C11	0.013 (2)	0.018 (2)	0.016 (2)	−0.0031 (19)	0.0017 (19)	−0.0048 (18)
C12	0.015 (2)	0.017 (2)	0.015 (2)	−0.0002 (19)	0.0038 (19)	−0.0005 (18)
C13	0.013 (2)	0.017 (2)	0.011 (2)	−0.0014 (18)	0.0018 (18)	0.0002 (17)

Geometric parameters (Å, º)

I1—C3	2.102 (5)	C2—C7	1.397 (7)
Co1—O2	2.077 (3)	C3—C4	1.393 (7)
Co1—O2ⁱ	2.077 (3)	C4—H4	0.9300
Co1—O4	2.135 (4)	C5—C4	1.383 (8)
Co1—O4ⁱ	2.135 (4)	C5—C6	1.383 (8)

Co1—N1	2.134 (4)	C5—H5	0.9300
Co1—N1[i]	2.134 (4)	C6—H6	0.9300
O1—C1	1.253 (6)	C7—C6	1.384 (7)
O2—C1	1.263 (6)	C7—H7	0.9300
O3—C13	1.235 (6)	C8—C9	1.390 (6)
O4—H41	0.855 (18)	C8—H8	0.9300
O4—H42	0.86 (2)	C9—C13	1.497 (7)
N1—C8	1.335 (7)	C10—C9	1.386 (7)
N1—C12	1.345 (6)	C10—C11	1.389 (7)
N2—C13	1.328 (6)	C10—H10	0.9300
N2—H21	0.86 (2)	C11—C12	1.381 (7)
N2—H22	0.86 (2)	C11—H11	0.9300
C2—C1	1.510 (7)	C12—H12	0.9300
C2—C3	1.396 (7)		
O2[i]—Co1—O2	180.0	C4—C3—I1	113.6 (4)
O2—Co1—N1	89.86 (14)	C4—C3—C2	121.3 (5)
O2[i]—Co1—N1	90.14 (14)	C3—C4—H4	120.3
O2—Co1—N1[i]	90.14 (14)	C5—C4—C3	119.4 (5)
O2[i]—Co1—N1[i]	89.86 (14)	C5—C4—H4	120.3
N1[i]—Co1—N1	180.0	C4—C5—H5	119.6
O2—Co1—O4	92.53 (14)	C6—C5—C4	120.8 (5)
O2[i]—Co1—O4	87.47 (14)	C6—C5—H5	119.6
O2—Co1—O4[i]	87.47 (14)	C5—C6—C7	119.0 (5)
O2[i]—Co1—O4[i]	92.53 (14)	C5—C6—H6	120.5
O4[i]—Co1—O4	180.00 (18)	C7—C6—H6	120.5
N1—Co1—O4	87.66 (15)	C2—C7—H7	119.0
N1[i]—Co1—O4	92.34 (15)	C6—C7—C2	122.1 (5)
N1—Co1—O4[i]	92.34 (15)	C6—C7—H7	119.0
N1[i]—Co1—O4[i]	87.66 (15)	N1—C8—C9	123.4 (5)
C1—O2—Co1	123.9 (3)	N1—C8—H8	118.3
Co1—O4—H41	120 (5)	C9—C8—H8	118.3
Co1—O4—H42	98 (5)	C8—C9—C13	117.9 (4)
H42—O4—H41	106 (4)	C10—C9—C8	117.8 (5)
C8—N1—Co1	119.2 (3)	C10—C9—C13	124.2 (4)
C8—N1—C12	118.2 (4)	C9—C10—C11	119.3 (5)
C12—N1—Co1	122.6 (3)	C9—C10—H10	120.3
C13—N2—H21	126 (5)	C11—C10—H10	120.3
C13—N2—H22	116 (5)	C10—C11—H11	120.5
H21—N2—H22	116 (7)	C12—C11—C10	118.9 (5)
O1—C1—O2	124.6 (5)	C12—C11—H11	120.5
O1—C1—C2	118.8 (4)	N1—C12—C11	122.3 (5)
O2—C1—C2	116.5 (4)	N1—C12—H12	118.8
C3—C2—C1	125.0 (4)	C11—C12—H12	118.8
C3—C2—C7	117.4 (5)	O3—C13—N2	122.6 (5)
C7—C2—C1	117.5 (4)	O3—C13—C9	120.0 (4)
C2—C3—I1	125.1 (4)	N2—C13—C9	117.4 (4)
N1—Co1—O2—C1	121.0 (4)	C1—C2—C3—I1	−0.8 (7)

N1ⁱ—Co1—O2—C1	−59.0 (4)	C1—C2—C3—C4	178.6 (5)
O4—Co1—O2—C1	33.4 (4)	C7—C2—C3—I1	−177.7 (3)
O4ⁱ—Co1—O2—C1	−146.6 (4)	C7—C2—C3—C4	1.7 (7)
O2—Co1—N1—C8	−135.9 (4)	C1—C2—C7—C6	−177.2 (5)
O2ⁱ—Co1—N1—C8	44.1 (4)	C3—C2—C7—C6	−0.1 (7)
O2—Co1—N1—C12	41.5 (4)	I1—C3—C4—C5	177.8 (4)
O2ⁱ—Co1—N1—C12	−138.5 (4)	C2—C3—C4—C5	−1.6 (8)
O4—Co1—N1—C8	−43.3 (4)	C6—C5—C4—C3	−0.1 (8)
O4ⁱ—Co1—N1—C8	136.7 (4)	C4—C5—C6—C7	1.7 (8)
O4—Co1—N1—C12	134.1 (4)	C2—C7—C6—C5	−1.6 (8)
O4ⁱ—Co1—N1—C12	−45.9 (4)	N1—C8—C9—C10	−0.4 (7)
Co1—O2—C1—O1	−19.5 (7)	N1—C8—C9—C13	176.6 (4)
Co1—O2—C1—C2	158.0 (3)	C8—C9—C13—O3	−6.2 (7)
Co1—N1—C8—C9	177.4 (4)	C8—C9—C13—N2	175.6 (5)
C12—N1—C8—C9	−0.2 (7)	C10—C9—C13—O3	170.7 (5)
Co1—N1—C12—C11	−176.4 (4)	C10—C9—C13—N2	−7.6 (8)
C8—N1—C12—C11	1.1 (7)	C11—C10—C9—C8	0.2 (7)
C3—C2—C1—O1	−21.1 (7)	C11—C10—C9—C13	−176.7 (5)
C3—C2—C1—O2	161.2 (5)	C9—C10—C11—C12	0.6 (8)
C7—C2—C1—O1	155.8 (5)	C10—C11—C12—N1	−1.3 (8)
C7—C2—C1—O2	−21.9 (6)		

Symmetry code: (i) −x, −y+1, −z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···O1ⁱⁱ	0.86 (6)	2.02 (6)	2.837 (6)	158 (5)
N2—H22···O3ⁱⁱⁱ	0.86 (6)	2.21 (7)	2.984 (7)	151 (7)
O4—H41···O3ⁱᵛ	0.86 (5)	2.00 (5)	2.827 (5)	162 (5)
O4—H42···O1	0.86 (5)	1.80 (6)	2.631 (5)	161 (7)
C10—H10···O1ⁱⁱ	0.93	2.51	3.400 (6)	160

Symmetry codes: (ii) *x*, *y*, *z*−1; (iii) −*x*+1, −*y*+1, −*z*−1; (iv) −*x*+1, −*y*+1, −*z*.