Crystal structure of *catena*-poly[[diaquabis(4-formylbenzoato-κO^1)cobalt(II)]-μ-pyrazine-$\kappa^2 N{:}N'$]

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In the title polymeric compound, $[Co(C_8H_5O_3)_2(C_4H_4N_2)(H_2O)_2]_n$, the Co^{II} atom is located on a twofold rotation axis and has a slightly distorted octahedral coordination sphere. In the equatorial plane, it is coordinated by two carboxylate O atoms of two symmetry-related monodentate formylbenzoate anions and by two N atoms of two bridging pyrazine ligands. The latter are bisected by the twofold rotation axis. The axial positions are occupied by two O atoms of the coordinating water molecules. In the formylbenzoate anion, the carboxylate group is twisted away from the attached benzene ring by 7.50 (8)°, while the benzene and pyrazine rings are oriented at a dihedral angle of 64.90 (4)°. The pyrazine ligands bridge the Co^{II} cations, forming linear chains running along the *b*-axis direction. Strong intramolecular O—H···O hydrogen bonds link the water molecules to the carboxylate O atoms. In the crystal, weak O—H$_{water}$···O$_{water}$ hydrogen bonds link adjacent chains into layers parallel to the *bc* plane. The layers are linked *via* C—H$_{pyrazine}$···O$_{formyl}$ hydrogen bonds, forming a three-dimensional network. There are also weak C—H···π interactions present.
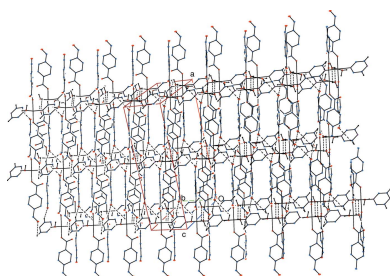
1. Chemical context

The structural functions and coordination relationships of the arylcarboxylate ion in transition metal complexes of benzoic acid derivatives change depending on the nature and position of the substituent groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of the synthesis (Adiwidjaja *et al.*, 1978; Antsyshkina *et al.*, 1980; Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981). Transition metal complexes with biochemically active ligands frequently show interesting physical and/or chemical properties and, as a result, they may find applications in biological systems (Antolini *et al.*, 1982). Some benzoic acid derivatives, such as 4-aminobenzoic acid, have been extensively reported in coordination chemistry, as bifunctional organic ligands, due to the varieties of their coordination modes (Chen & Chen, 2002; Amiraslanov *et al.*, 1979; Hauptmann *et al.*, 2000).

In this context, we report the synthesis and crystal structure of the title compound, $[Co(C_8H_5O_3)_2(C_4H_4N_2)(H_2O)_2]_n$, which is isotypic with its Cu^{II} (Çelik *et al.*, 2014*a*) and Ni^{II} (Çelik *et al.*, 2014*b*) analogues.

2. Structural commentary

The asymmetric unit of the title compound contains a Co^{II} ion, one formylbenzoate (FB) anion, one water molecule and half of a pyrazine molecule. Atoms N1 and N2 of the pyrazine

ligand and Co1 are located on a twofold rotation axis (Fig. 1). The pyrazine ligands bridge adjacent Co^{II} ions, forming polymeric chains running along the b-axis direction (Fig. 2). The distance between symmetry-related Co^{II} ions [Co1$\cdots$Co1^{iii}; symmetry code: (iii) $x, y + 1, z$] is 7.1193 (4) Å.

The equatorial plane of the $Co^{II}O_4N_2$ coordination sphere is composed of two carboxylate O atoms [O1 and O1^i; symmetry code: (i) $2 - x, y, \frac{3}{2} - z$] of two symmetry-related monodentate formylbenzoate anions and two N atoms [N1 and N2^{ii}; symmetry code: (ii) $x, -1 + y, z$] of two bridging pyrazine ligands, which are bisected by the twofold rotation axis. The axial positions are occupied by two O atoms (O4 and O4^i) of the coordinating water molecules.

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

$Cg1$ is the centroid of ring A (C2–C7).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H41$\cdots$O2	0.89 (3)	1.72 (3)	2.5909 (16)	164 (2)
O4—H42$\cdots$O4^i	0.71 (3)	2.63 (3)	2.958 (2)	111 (2)
C10—H10$\cdots$O3^{ii}	0.93	2.46	3.320 (2)	154
C7—H7$\cdots$Cg1^{iii}	0.93	2.65	3.4216 (15)	142

Symmetry codes: (i) $-x + 2, -y, -z + 1$; (ii) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 2$; (iii) $x, -y, z - \frac{1}{2}$.

The near equality of the C1—O1 [1.272 (2) Å] and C1—O2 [1.245 (2) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds. The Co—N bond length is 2.165 (9) Å, while the Co—O bond lengths are 2.0551 (9) Å (for benzoate oxygen) and 2.1491 (11) Å (for water oxygen), close to standard values. The Co1 atom is displaced by 0.1034 (2) Å from the mean plane of the carboxylate group (O1/C1/O2). The dihedral angle between the carboxylate group and the adjacent benzene ring A (C2–C7) is 7.50 (8)°, while the benzene and pyrazine rings are oriented at a dihedral angle of 64.90 (4)°.

3. Supramolecular features

Strong intramolecular O—H$\cdots$O hydrogen bonds (Table 1) link the water molecules to the non-coordinating carboxylate oxygen atoms. In the crystal, weak O—H$_{water}\cdots$O$_{water}$ hydrogen bonds (Table 1) link adjacent chains into layers parallel to the bc plane. The layers are linked *via* C—H$_{pyrazine}\cdots$O$_{formyl}$ hydrogen bonds, forming a three-dimensional network (Fig. 3). There are also weak C—H$\cdots\pi$ interactions present (Table 1).
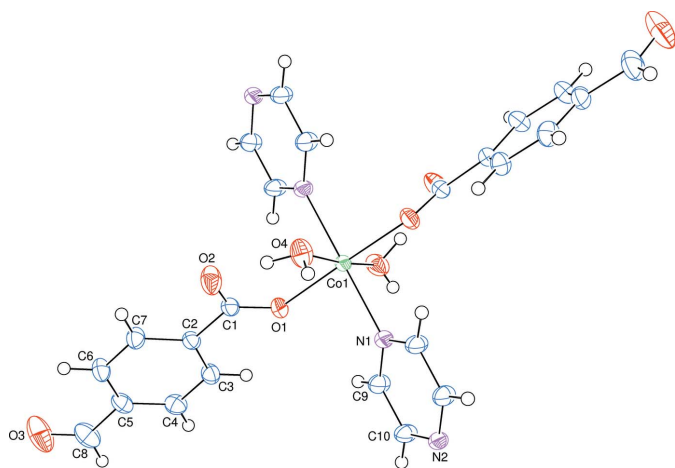

Figure 1
A view of the coordination environment around the Co^{II} atom of the title molecule, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The twofold rotation axis bisects atoms Co1, N1 and N2. Non-labelled atoms are generated by the symmetry code $-x + 2, y, -z + \frac{3}{2}$.
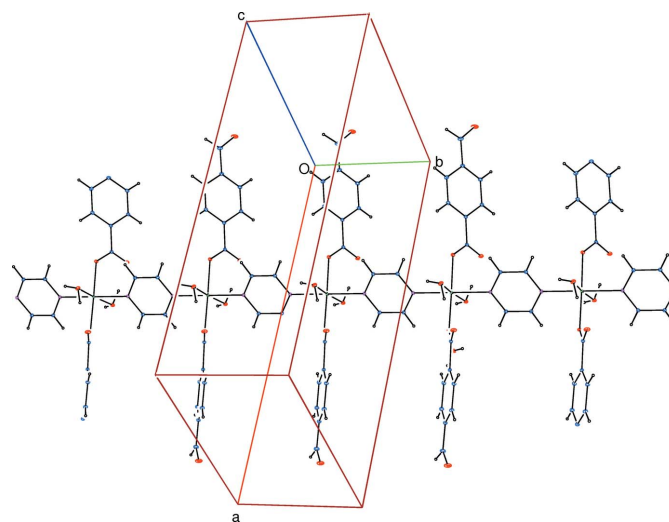
Figure 2
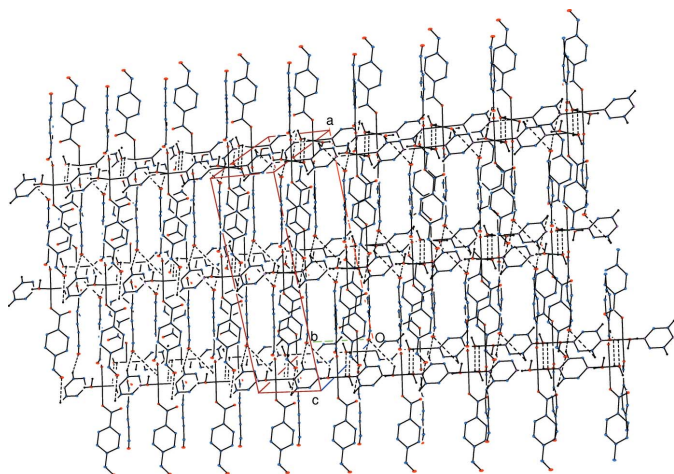A partial view of the crystal packing of the title compound.

Figure 3
Part of the crystal structure. Intermolecular hydrogen bonds are shown as dashed lines. Non-bonding H atoms have been omitted for clarity.

4. Refinement

The experimental details including the crystal data, data collection and refinement are summarized in Table 2. Atoms H41 and H42 (for H_2O) were located in a difference Fourier map and were refined freely. The methine H atom was also located in a difference Fourier map and the C—H distance restrained to 0.984 (13) Å. The aromatic C-bound H atoms were positioned geometrically with C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

5. Synthesis and crystallization

The title compound was prepared by the reaction of $CoSO_4 \cdot 7H_2O$ (1.40 g, 5 mmol) in H_2O (25 ml) and pyrazine (0.40 g, 5 mmol) in H_2O (25 ml) with sodium 4-formyl-benzoate (1.72 g, 10 mmol) in H_2O (70 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving orange single crystals.

Acknowledgements

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_8H_5O_3)_2(C_4H_4N_2)(H_2O)_2]$
M_r	473.29
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	296
a, b, c (Å)	22.1623 (6), 7.1193 (2), 12.2911 (3)
β (°)	94.432 (1)
V (Å^3)	1933.49 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.94
Crystal size (mm)	$0.47 \times 0.22 \times 0.11$
Data collection	
Diffractometer	Bruker SMART BREEZE CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.830, 0.914
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27023, 2427, 2336
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.071, 1.06
No. of reflections	2427
No. of parameters	154
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.34

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3* for Windows and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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supporting information

Crystal structure of *catena*-poly[[diaquabis(4-formylbenzoato-*κO*¹)cobalt(II)]-*μ*-pyrazine-*κ²N:N′*]

Gülçin Şefiye Aşkın, Fatih Çelik, Nefise Dilek, Hacali Necefoğlu and Tuncer Hökelek

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); 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); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

catena-**Poly[[diaquabis(4-formylbenzoato-*κO*¹)cobalt(II)]-*μ*-pyrazine-*κ²N:N′*]**

Crystal data

[Co(C₈H₅O₃)₂(C₄H₄N₂)(H₂O)₂]	$F(000) = 972$
$M_r = 473.29$	$D_x = 1.626$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 9866 reflections
$a = 22.1623\ (6)$ Å	$\theta = 2.4–28.3°$
$b = 7.1193\ (2)$ Å	$\mu = 0.94$ mm^{-1}
$c = 12.2911\ (3)$ Å	$T = 296$ K
$\beta = 94.432\ (1)°$	Block, orange
$V = 1933.49\ (9)$ Å³	$0.47 \times 0.22 \times 0.11$ mm
$Z = 4$	

Data collection

Bruker SMART BREEZE CCD diffractometer	27023 measured reflections
Radiation source: fine-focus sealed tube	2427 independent reflections
Graphite monochromator	2336 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.024$
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)	$\theta_{max} = 28.4°$, $\theta_{min} = 1.8°$
	$h = -29 \rightarrow 29$
	$k = -9 \rightarrow 9$
$T_{min} = 0.830$, $T_{max} = 0.914$	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.025$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.071$	
$S = 1.06$	Hydrogen site location: inferred from neighbouring sites
2427 reflections	
154 parameters	H atoms treated by a mixture of independent and constrained refinement
1 restraint	

$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 1.5712P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.0000	−0.05145 (3)	0.7500	0.01998 (9)
O1	0.91572 (4)	−0.04830 (13)	0.80894 (9)	0.0276 (2)
O2	0.86274 (5)	−0.17780 (18)	0.66579 (9)	0.0402 (3)
O3	0.60114 (6)	−0.1312 (3)	0.95577 (12)	0.0651 (4)
O4	0.96115 (5)	−0.06701 (18)	0.58454 (9)	0.0352 (2)
H41	0.9245 (12)	−0.104 (4)	0.600 (2)	0.058 (6)*
H42	0.9564 (12)	0.019 (4)	0.555 (2)	0.066 (8)*
N1	1.0000	0.2518 (2)	0.7500	0.0247 (3)
N2	1.0000	0.6436 (2)	0.7500	0.0235 (3)
C1	0.86731 (5)	−0.11157 (17)	0.75983 (11)	0.0240 (2)
C2	0.81095 (5)	−0.10250 (17)	0.82116 (10)	0.0226 (2)
C3	0.81105 (6)	−0.0089 (2)	0.92052 (11)	0.0268 (2)
H3	0.8467	0.0439	0.9518	0.032*
C4	0.75794 (6)	0.0058 (2)	0.97289 (11)	0.0301 (3)
H4	0.7580	0.0682	1.0394	0.036*
C5	0.70463 (6)	−0.0726 (2)	0.92617 (12)	0.0292 (3)
C6	0.70446 (6)	−0.1685 (2)	0.82755 (12)	0.0307 (3)
H6	0.6689	−0.2222	0.7967	0.037*
C7	0.75745 (6)	−0.18340 (19)	0.77557 (11)	0.0271 (3)
H7	0.7574	−0.2478	0.7098	0.032*
C8	0.64849 (8)	−0.0553 (3)	0.98296 (15)	0.0430 (4)
H8	0.6472 (7)	0.029 (2)	1.0463 (12)	0.021 (4)*
C9	0.97461 (6)	0.35053 (18)	0.82681 (11)	0.0287 (3)
H9	0.9563	0.2869	0.8815	0.034*
C10	0.97486 (7)	0.54530 (17)	0.82719 (12)	0.0282 (3)
H10	0.9571	0.6090	0.8825	0.034*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01683 (12)	0.01603 (12)	0.02763 (14)	0.000	0.00520 (8)	0.000
O1	0.0180 (4)	0.0288 (5)	0.0366 (5)	−0.0022 (3)	0.0058 (4)	−0.0040 (4)

O2	0.0284 (5)	0.0584 (7)	0.0351 (5)	−0.0116 (5)	0.0103 (4)	−0.0128 (5)
O3	0.0296 (6)	0.1092 (13)	0.0583 (8)	−0.0015 (7)	0.0149 (5)	0.0049 (9)
O4	0.0299 (5)	0.0449 (6)	0.0312 (5)	−0.0052 (5)	0.0051 (4)	0.0083 (5)
N1	0.0217 (7)	0.0178 (6)	0.0353 (8)	0.000	0.0065 (6)	0.000
N2	0.0242 (7)	0.0172 (6)	0.0301 (7)	0.000	0.0078 (6)	0.000
C1	0.0197 (5)	0.0204 (5)	0.0324 (6)	−0.0004 (4)	0.0059 (4)	0.0013 (5)
C2	0.0193 (5)	0.0218 (5)	0.0270 (6)	0.0006 (4)	0.0039 (4)	0.0022 (4)
C3	0.0224 (6)	0.0303 (6)	0.0272 (6)	0.0003 (5)	−0.0008 (5)	−0.0012 (5)
C4	0.0312 (7)	0.0337 (7)	0.0259 (6)	0.0040 (6)	0.0048 (5)	−0.0022 (5)
C5	0.0236 (6)	0.0332 (7)	0.0317 (6)	0.0046 (5)	0.0086 (5)	0.0055 (5)
C6	0.0207 (6)	0.0367 (7)	0.0351 (7)	−0.0048 (5)	0.0038 (5)	−0.0002 (6)
C7	0.0234 (6)	0.0308 (6)	0.0274 (6)	−0.0050 (5)	0.0048 (5)	−0.0036 (5)
C8	0.0316 (8)	0.0576 (11)	0.0417 (8)	0.0079 (7)	0.0152 (6)	0.0035 (7)
C9	0.0318 (6)	0.0211 (6)	0.0349 (7)	−0.0002 (5)	0.0137 (5)	0.0036 (5)
C10	0.0332 (7)	0.0210 (6)	0.0321 (7)	0.0016 (5)	0.0141 (5)	−0.0009 (5)

Geometric parameters (Å, º)

Co1—O1	2.0551 (9)	C2—C1	1.5093 (17)
Co1—O1[i]	2.0551 (9)	C2—C3	1.3911 (18)
Co1—O4	2.1491 (11)	C2—C7	1.3961 (17)
Co1—O4[i]	2.1491 (11)	C3—H3	0.9300
Co1—N1	2.1588 (15)	C4—C3	1.3884 (18)
Co1—N2[ii]	2.1714 (15)	C4—H4	0.9300
O1—C1	1.2721 (16)	C5—C4	1.390 (2)
O2—C1	1.2451 (17)	C5—C6	1.391 (2)
O3—C8	1.205 (2)	C5—C8	1.478 (2)
O4—H41	0.89 (3)	C6—H6	0.9300
O4—H42	0.71 (3)	C7—C6	1.3836 (18)
N1—C9	1.3357 (15)	C7—H7	0.9300
N1—C9[i]	1.3357 (15)	C8—H8	0.984 (13)
N2—Co1[iii]	2.1714 (15)	C9—H9	0.9300
N2—C10	1.3347 (15)	C10—C9	1.3866 (19)
N2—C10[i]	1.3347 (15)	C10—H10	0.9300
O1—Co1—O1[i]	178.75 (5)	C3—C2—C1	120.92 (11)
O1—Co1—O4	91.46 (4)	C3—C2—C7	119.58 (12)
O1[i]—Co1—O4	88.60 (4)	C7—C2—C1	119.46 (11)
O1—Co1—O4[i]	88.60 (4)	C2—C3—H3	120.0
O1[i]—Co1—O4[i]	91.46 (4)	C4—C3—C2	119.94 (12)
O1—Co1—N1	89.38 (3)	C4—C3—H3	120.0
O1[i]—Co1—N1	89.38 (3)	C3—C4—C5	120.15 (13)
O1—Co1—N2[ii]	90.62 (3)	C3—C4—H4	119.9
O1[i]—Co1—N2[ii]	90.62 (3)	C5—C4—H4	119.9
O4—Co1—O4[i]	174.09 (7)	C4—C5—C6	120.13 (12)
O4—Co1—N1	92.96 (4)	C4—C5—C8	119.41 (14)
O4[i]—Co1—N1	92.96 (4)	C6—C5—C8	120.46 (14)
O4—Co1—N2[ii]	87.04 (4)	C5—C6—H6	120.2

O4^{i}—Co1—N2^{ii}	87.04 (4)	C7—C6—C5	119.67 (12)
N1—Co1—N2^{ii}	180.000 (1)	C7—C6—H6	120.2
C1—O1—Co1	125.81 (9)	C2—C7—H7	119.7
Co1—O4—H41	96.6 (15)	C6—C7—C2	120.52 (12)
Co1—O4—H42	118 (2)	C6—C7—H7	119.7
H41—O4—H42	105 (3)	O3—C8—C5	125.34 (17)
C9—N1—Co1	121.75 (8)	O3—C8—H8	114.5 (10)
C9^{i}—N1—Co1	121.75 (8)	C5—C8—H8	120.1 (10)
C9—N1—C9^{i}	116.49 (15)	N1—C9—C10	121.79 (12)
C10—N2—Co1^{iii}	121.61 (8)	N1—C9—H9	119.1
C10^{i}—N2—Co1^{iii}	121.61 (8)	C10—C9—H9	119.1
C10—N2—C10^{i}	116.79 (15)	N2—C10—C9	121.57 (12)
O1—C1—C2	116.62 (11)	N2—C10—H10	119.2
O2—C1—O1	125.42 (12)	C9—C10—H10	119.2
O2—C1—C2	117.96 (11)		
O4—Co1—O1—C1	23.45 (11)	C3—C2—C1—O1	7.53 (18)
O4^{i}—Co1—O1—C1	−150.64 (11)	C3—C2—C1—O2	−171.75 (13)
N1—Co1—O1—C1	116.39 (10)	C7—C2—C1—O1	−174.80 (12)
N2^{ii}—Co1—O1—C1	−63.61 (10)	C7—C2—C1—O2	5.92 (18)
O1—Co1—N1—C9	35.39 (8)	C1—C2—C3—C4	176.79 (12)
O1^{i}—Co1—N1—C9	−144.61 (8)	C7—C2—C3—C4	−0.9 (2)
O1—Co1—N1—C9^{i}	−144.61 (8)	C1—C2—C7—C6	−176.64 (12)
O1^{i}—Co1—N1—C9^{i}	35.39 (8)	C3—C2—C7—C6	1.1 (2)
O4—Co1—N1—C9	126.82 (8)	C5—C4—C3—C2	−0.1 (2)
O4^{i}—Co1—N1—C9	−53.18 (8)	C4—C5—C6—C7	−0.8 (2)
O4—Co1—N1—C9^{i}	−53.18 (8)	C6—C5—C4—C3	1.0 (2)
O4^{i}—Co1—N1—C9^{i}	126.82 (8)	C8—C5—C4—C3	−179.86 (14)
Co1—O1—C1—O2	−3.6 (2)	C8—C5—C6—C7	−179.95 (14)
Co1—O1—C1—C2	177.23 (8)	C4—C5—C8—O3	−172.93 (18)
Co1—N1—C9—C10	179.66 (10)	C6—C5—C8—O3	6.3 (3)
C9^{i}—N1—C9—C10	−0.34 (10)	C2—C7—C6—C5	−0.2 (2)
Co1^{iii}—N2—C10—C9	179.66 (10)	N2—C10—C9—N1	0.7 (2)
C10^{i}—N2—C10—C9	−0.34 (10)		

Symmetry codes: (i) −x+2, y, −z+3/2; (ii) x, y−1, z; (iii) x, y+1, z.

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of ring A (C2–C7).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O4—H41⋯O2	0.89 (3)	1.72 (3)	2.5909 (16)	164 (2)
O4—H42⋯O4^{iv}	0.71 (3)	2.63 (3)	2.958 (2)	111 (2)
C10—H10⋯O3^{v}	0.93	2.46	3.320 (2)	154
C7—H7⋯Cg1^{vi}	0.93	2.65	3.4216 (15)	142

Symmetry codes: (iv) −x+2, −y, −z+1; (v) −x+3/2, −y+1/2, −z+2; (vi) x, −y, z−1/2.