metal-organic compounds

Tetraaquabis(isonicotinamide-κN^1)-cobalt(II) bis(4-formylbenzoate) dihydrate

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The asymmetric unit of the crystal structure of the title complex, [Co(C$_6$H$_6$N$_2$O)$_2$(H$_2$O)$_4$](C$_8$H$_5$O$_3$)$_2$·2H$_2$O, contains one-half of the complex cation with the Co^{II} ion located on an inversion center, a 4-formylbenzoate (FB) counter-anion and an uncoordinated water molecule. The four O atoms in the equatorial plane around the Co^{II} ion form a slightly distorted square-planar arrangement with an average Co—O bond length of 2.086 Å; the slightly distorted octahedral coordination is completed by the two N atoms of the isonicotinamide (INA) ligands at a slightly longer distance [2.1603 (14) Å] in the axial positions. The dihedral angle between the carboxylate group and the attached benzene ring is 5.93 (13)°, while the pyridine and benzene rings are oriented at a dihedral angle of 3.09 (6)°. In the crystal structure, O—H···O, N—H···O and C—H···O hydrogen bonds link the molecules into a three-dimensional network. π–π Contacts between the benzene and pyridine rings [centroid–centroid distance = 3.758 (1) Å] may further stabilize the crystal structure.

Related literature

For general background to transition metal complexes of nicotinamide and/or the nicotinic acid derivative *N,N*-diethylnicotinamide, see: Bigoli *et al.* (1972); Krishnamachari (1974). For related structures, see: Hökelek *et al.* (2009); Sertçelik *et al.* (2009).
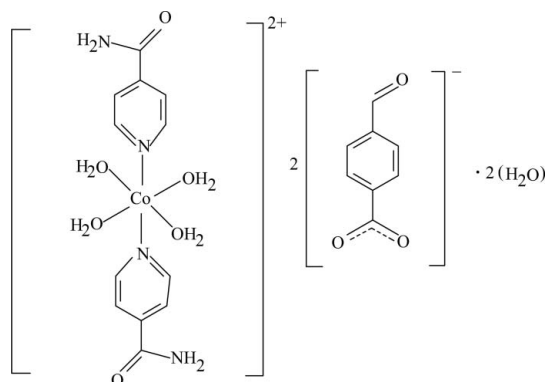
Experimental

Crystal data

[Co(C$_6$H$_6$N$_2$O)$_2$(H$_2$O)$_4$](C$_8$H$_5$O$_3$)$_2$·2H$_2$O	β = 84.681 (3)°
M_r = 709.53	γ = 72.564 (2)°
Triclinic, $P\bar{1}$	V = 761.28 (5) Å^3
a = 6.4490 (2) Å	Z = 1
b = 6.8836 (3) Å	Mo $K\alpha$ radiation
c = 18.1792 (5) Å	μ = 0.64 mm^{-1}
α = 81.967 (3)°	T = 100 K
	0.17 × 0.08 × 0.04 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	13740 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	3780 independent reflections
T_{min} = 0.943, T_{max} = 0.978	2884 reflections with $I > 2\sigma(I)$
	R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.074	
S = 0.98	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
3780 reflections	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
236 parameters	
9 restraints	

Table 1
Selected bond lengths (Å).

Co1—O5	2.0570 (13)	Co1—N1	2.1603 (14)
Co1—O6	2.1151 (12)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^i	0.86	2.13	2.9680 (19)	166
N2—H2B···O7^{ii}	0.86	2.05	2.8659 (19)	158
O5—H51···O1^{iii}	0.916 (18)	1.723 (18)	2.6355 (18)	174.5 (18)
O5—H52···O2	0.868 (15)	1.863 (15)	2.7236 (18)	171.1 (18)
O6—H61···O1^{iv}	0.899 (15)	1.872 (15)	2.7707 (19)	177.3 (11)
O6—H62···O2^v	0.87 (2)	1.92 (2)	2.7760 (19)	168 (2)
O7—H71···O3^{vi}	0.891 (19)	1.850 (18)	2.7371 (19)	173.7 (18)
O7—H72···O4^i	0.936 (15)	1.982 (15)	2.9168 (19)	176.8 (17)
C9—H9···O7^{ii}	0.93	2.56	3.458 (2)	161
C12—H12···O5^{vii}	0.93	2.45	3.210 (2)	139

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

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: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2594).

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supplementary materials

Tetraaquabis(isonicotinamide-κN^1)cobalt(II) bis(4-formylbenzoate) dihydrate

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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 is a monomeric complex, with Co^{II} ion on a centre of symmetry, consisting of two INA ligands, four coordinated water molecules, two FB anions and two uncoordinated water molecules. The structures of some DENA and/or INA complexes of Co^{II} ion, [Co(C$_8$H$_5$O$_3$)$_2$(C$_{10}$H$_{14}$N$_2$O)$_2$(H$_2$O)$_2$] (Sertçelik *et al.*, 2009) and [Co(C$_6$H$_6$N$_2$O)(C$_9$H$_{10}$NO$_2$)$_2$(H$_2$O)$_2$] (Hökelek *et al.*, 2009) have also been determined.

In the title compound, INA ligands are monodentate. The four O atoms (O5, O6, and the symmetry-related atoms, O5', O6') in the equatorial plane around the Co atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two pyridine N atoms (N1, N1') of the INA ligands at 2.1603 (14) Å from the Co atom in the axial positions (Table 1, Fig. 1). The average Co—O bond length is 2.0861 (13) Å. The O—H···O hydrogen bond (Table 2) links the coordinated water molecule to the FB anion. The dihedral angle between the planar carboxylate group (O1/O2/C1) and the benzene ring A (C2—C7) is 5.93 (13)°, while that between rings A and B (N1/C8—C12) is 3.09 (6)°.

In the crystal structure, O—H···O, N—H···O and C—H···O hydrogen bonds (Table 2) link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the structure. The π–π contact between the benzene and pyridine rings, *Cg*1—*Cg*2, [where *Cg*1 and *Cg*2 are centroids of the rings A (C2—C7) and B (N1/C8—C12), respectively] may further stabilize the structure, with centroid-centroid distance of 3.758 (1) Å.

Experimental

The title compound was prepared by the reaction of CoSO$_4$.7H$_2$O (1.41 g, 5 mmol) in H$_2$O (25 ml) and INA (1.22 g, 10 mmol) in H$_2$O (40 ml) with sodium 4-formylbenzoate (1.72 g, 10 mmol) in H$_2$O (50 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving orange single crystals.

Refinement

Atoms H51, H52, H61, H62, H71 and H72 (for H$_2$O) and H14 (for CH) were located in difference Fourier map and refined isotropically, with restrains of O5—H51 = 0.916 (13), O5—H52 = 0.865 (14), O6—H61 = 0.899 (13), O6—H62 = 0.871 (14), O7—H71 = 0.892 (14), O7—H72 = 0.935 (13) Å and H51—O5—H52 = 106.6 (16), H61—O6—H62 = 106.4 (16), H71—O7—H72 = 106.5 (15) °. The remaining H atoms were positioned geometrically with N—H = 0.86 Å (for NH$_2$) and 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,N).

supplementary materials

Figures

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

Tetraaquabis(isonicotinamide-κ*N*[1])cobalt(II) bis(4-formylbenzoate) dihydrate

Crystal data

$[Co(C_6H_6N_2O)_2(H_2O)_4](C_8H_5O_3)_2 \cdot 2H_2O$	$Z = 1$
$M_r = 709.53$	$F_{000} = 369$
Triclinic, $P\bar{1}$	$D_x = 1.548$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.4490$ (2) Å	Cell parameters from 4050 reflections
$b = 6.8836$ (3) Å	$\theta = 1.1–28.4°$
$c = 18.1792$ (5) Å	$\mu = 0.64$ mm^{-1}
$\alpha = 81.967$ (3)°	$T = 100$ K
$\beta = 84.681$ (3)°	Rod-shaped, orange
$\gamma = 72.564$ (2)°	$0.17 \times 0.08 \times 0.04$ mm
$V = 761.28$ (5) Å^3	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	3780 independent reflections
Radiation source: fine-focus sealed tube	2884 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.054$
$T = 100$ K	$\theta_{max} = 28.4°$
φ and ω scans	$\theta_{min} = 1.1°$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -8 \rightarrow 8$
$T_{min} = 0.943$, $T_{max} = 0.978$	$k = -9 \rightarrow 8$
13740 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.074$	$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
3780 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}

236 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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	0.0000	0.0000	0.0000	0.01071 (11)
O1	−0.3206 (2)	0.68183 (19)	−0.08763 (7)	0.0168 (3)
O2	0.0316 (2)	0.55083 (19)	−0.12091 (7)	0.0154 (3)
O3	0.6316 (2)	−0.2347 (2)	0.31750 (7)	0.0191 (3)
O4	−0.5540 (2)	0.7430 (2)	−0.46372 (7)	0.0249 (3)
O5	0.1816 (2)	0.2025 (2)	−0.02613 (7)	0.0129 (3)
H51	0.226 (3)	0.251 (3)	0.0122 (9)	0.015*
H52	0.122 (3)	0.309 (2)	−0.0568 (9)	0.015*
O6	0.2398 (2)	−0.2399 (2)	−0.04719 (7)	0.0154 (3)
H61	0.382 (2)	−0.268 (3)	−0.0613 (10)	0.015*
H62	0.189 (3)	−0.321 (3)	−0.0685 (10)	0.015*
O7	0.1474 (2)	0.1218 (2)	0.58230 (7)	0.0212 (3)
H71	0.222 (3)	0.165 (3)	0.6122 (9)	0.015*
H72	0.239 (3)	−0.002 (2)	0.5679 (10)	0.015*
N1	0.1381 (2)	−0.0933 (2)	0.10768 (8)	0.0118 (3)
N2	0.3064 (2)	−0.1744 (2)	0.38109 (8)	0.0159 (4)
H2A	0.3647	−0.1901	0.4230	0.019*
H2B	0.1675	−0.1461	0.3796	0.019*
C1	−0.1665 (3)	0.6195 (3)	−0.13455 (10)	0.0133 (4)
C2	−0.2240 (3)	0.6309 (3)	−0.21448 (10)	0.0119 (4)
C3	−0.0588 (3)	0.5837 (3)	−0.26939 (10)	0.0149 (4)
H3	0.0859	0.5438	−0.2570	0.018*
C4	−0.1087 (3)	0.5957 (3)	−0.34277 (10)	0.0164 (4)
H4	0.0023	0.5630	−0.3795	0.020*
C5	−0.3246 (3)	0.6567 (3)	−0.36142 (10)	0.0150 (4)
C6	−0.4913 (3)	0.7031 (3)	−0.30633 (10)	0.0146 (4)
H6	−0.6359	0.7427	−0.3187	0.018*
C7	−0.4407 (3)	0.6900 (3)	−0.23320 (10)	0.0140 (4)
H7	−0.5517	0.7206	−0.1964	0.017*

C8	0.0137 (3)	−0.0686 (3)	0.17118 (10)	0.0130 (4)
H8	−0.1367	−0.0279	0.1683	0.016*
C9	0.0981 (3)	−0.1008 (3)	0.24058 (10)	0.0128 (4)
H9	0.0057	−0.0807	0.2830	0.015*
C10	0.3216 (3)	−0.1633 (3)	0.24610 (10)	0.0114 (4)
C11	0.4511 (3)	−0.1974 (3)	0.18124 (10)	0.0137 (4)
H11	0.6018	−0.2448	0.1830	0.016*
C12	0.3547 (3)	−0.1602 (3)	0.11403 (10)	0.0146 (4)
H12	0.4440	−0.1827	0.0710	0.018*
C13	0.4314 (3)	−0.1941 (3)	0.31843 (10)	0.0132 (4)
C14	−0.3744 (3)	0.6684 (3)	−0.43957 (11)	0.0203 (5)
H14	−0.251 (3)	0.611 (3)	−0.4732 (11)	0.025 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0088 (2)	0.0147 (2)	0.00937 (19)	−0.00406 (16)	−0.00113 (14)	−0.00213 (14)
O1	0.0131 (7)	0.0241 (8)	0.0145 (7)	−0.0058 (6)	−0.0016 (5)	−0.0053 (6)
O2	0.0110 (7)	0.0181 (7)	0.0175 (7)	−0.0034 (6)	−0.0053 (5)	−0.0027 (6)
O3	0.0116 (7)	0.0274 (8)	0.0181 (7)	−0.0028 (6)	−0.0042 (6)	−0.0068 (6)
O4	0.0248 (8)	0.0311 (9)	0.0159 (7)	−0.0013 (7)	−0.0082 (6)	−0.0036 (6)
O5	0.0124 (7)	0.0173 (7)	0.0101 (7)	−0.0054 (6)	−0.0040 (5)	−0.0007 (5)
O6	0.0100 (7)	0.0195 (8)	0.0186 (7)	−0.0049 (6)	0.0001 (6)	−0.0078 (6)
O7	0.0157 (8)	0.0304 (9)	0.0191 (7)	−0.0062 (7)	−0.0028 (6)	−0.0079 (6)
N1	0.0107 (8)	0.0134 (8)	0.0123 (8)	−0.0047 (7)	−0.0004 (6)	−0.0021 (6)
N2	0.0137 (8)	0.0243 (9)	0.0106 (8)	−0.0048 (7)	−0.0051 (6)	−0.0033 (7)
C1	0.0166 (10)	0.0101 (10)	0.0147 (9)	−0.0058 (8)	−0.0034 (8)	−0.0011 (7)
C2	0.0132 (10)	0.0095 (9)	0.0138 (9)	−0.0041 (8)	−0.0028 (7)	−0.0006 (7)
C3	0.0114 (10)	0.0148 (10)	0.0185 (10)	−0.0031 (8)	−0.0032 (8)	−0.0024 (8)
C4	0.0154 (10)	0.0163 (10)	0.0155 (10)	−0.0024 (8)	0.0017 (8)	−0.0020 (8)
C5	0.0193 (10)	0.0133 (10)	0.0126 (9)	−0.0045 (8)	−0.0025 (8)	−0.0012 (8)
C6	0.0114 (10)	0.0160 (10)	0.0166 (10)	−0.0033 (8)	−0.0042 (8)	−0.0018 (8)
C7	0.0138 (10)	0.0132 (10)	0.0146 (9)	−0.0029 (8)	−0.0001 (8)	−0.0028 (8)
C8	0.0091 (9)	0.0152 (10)	0.0140 (9)	−0.0023 (8)	−0.0018 (7)	−0.0015 (8)
C9	0.0122 (10)	0.0160 (10)	0.0104 (9)	−0.0048 (8)	0.0010 (7)	−0.0022 (7)
C10	0.0141 (10)	0.0085 (9)	0.0127 (9)	−0.0038 (8)	−0.0039 (7)	−0.0014 (7)
C11	0.0089 (9)	0.0168 (10)	0.0161 (10)	−0.0040 (8)	−0.0032 (7)	−0.0021 (8)
C12	0.0108 (10)	0.0190 (10)	0.0136 (9)	−0.0036 (8)	0.0005 (7)	−0.0028 (8)
C13	0.0147 (10)	0.0112 (10)	0.0143 (9)	−0.0031 (8)	−0.0035 (8)	−0.0027 (7)
C14	0.0236 (12)	0.0214 (11)	0.0143 (10)	−0.0039 (10)	0.0002 (9)	−0.0033 (9)

Geometric parameters (Å, °)

Co1—O5	2.0570 (13)	C2—C3	1.387 (2)
Co1—O5^i	2.0570 (13)	C3—C4	1.387 (2)
Co1—O6	2.1151 (12)	C3—H3	0.9300
Co1—O6^i	2.1151 (12)	C4—H4	0.9300
Co1—N1	2.1603 (14)	C5—C4	1.388 (3)

Co1—N1[i]	2.1603 (14)	C5—C14	1.471 (3)
O1—C1	1.261 (2)	C6—C5	1.394 (2)
O2—C1	1.257 (2)	C6—C7	1.382 (2)
O3—C13	1.236 (2)	C6—H6	0.9300
O4—C14	1.214 (2)	C7—C2	1.394 (2)
O5—H51	0.916 (13)	C7—H7	0.9300
O5—H52	0.865 (14)	C8—H8	0.9300
O6—H61	0.899 (13)	C9—C8	1.383 (2)
O6—H62	0.871 (14)	C9—C10	1.384 (2)
O7—H71	0.892 (14)	C9—H9	0.9300
O7—H72	0.935 (13)	C10—C11	1.386 (2)
N1—C8	1.344 (2)	C10—C13	1.510 (2)
N1—C12	1.344 (2)	C11—C12	1.380 (2)
N2—C13	1.331 (2)	C11—H11	0.9300
N2—H2A	0.8600	C12—H12	0.9300
N2—H2B	0.8600	C14—H14	0.976 (19)
C2—C1	1.518 (2)		
O5—Co1—O5[i]	180.00 (4)	C4—C3—C2	120.16 (17)
O5—Co1—O6	93.11 (5)	C4—C3—H3	119.9
O5[i]—Co1—O6	86.89 (5)	C3—C4—C5	119.95 (17)
O5—Co1—O6[i]	86.89 (5)	C3—C4—H4	120.0
O5[i]—Co1—O6[i]	93.11 (5)	C5—C4—H4	120.0
O5—Co1—N1	90.50 (5)	C4—C5—C6	120.09 (16)
O5[i]—Co1—N1	89.50 (5)	C4—C5—C14	119.15 (17)
O5—Co1—N1[i]	89.50 (5)	C6—C5—C14	120.75 (17)
O5[i]—Co1—N1[i]	90.50 (5)	C5—C6—H6	120.1
O6—Co1—O6[i]	180.00 (9)	C7—C6—C5	119.78 (17)
O6—Co1—N1	91.81 (5)	C7—C6—H6	120.1
O6[i]—Co1—N1	88.19 (5)	C2—C7—H7	119.9
O6—Co1—N1[i]	88.19 (5)	C6—C7—C2	120.21 (17)
O6[i]—Co1—N1[i]	91.81 (5)	C6—C7—H7	119.9
N1[i]—Co1—N1	180.00 (3)	N1—C8—C9	123.34 (16)
Co1—O5—H51	118.1 (12)	N1—C8—H8	118.3
Co1—O5—H52	114.2 (12)	C9—C8—H8	118.3
H51—O5—H52	106.5 (16)	C8—C9—C10	119.24 (16)
Co1—O6—H61	136.9 (12)	C8—C9—H9	120.4
Co1—O6—H62	114.8 (12)	C10—C9—H9	120.4
H62—O6—H61	106.4 (16)	C9—C10—C11	117.81 (16)
H71—O7—H72	106.5 (15)	C9—C10—C13	123.74 (16)
C8—N1—Co1	121.76 (12)	C11—C10—C13	118.44 (16)
C12—N1—Co1	121.13 (12)	C10—C11—H11	120.3
C12—N1—C8	116.80 (15)	C12—C11—C10	119.46 (17)
C13—N2—H2A	120.0	C12—C11—H11	120.3
C13—N2—H2B	120.0	N1—C12—C11	123.26 (16)
H2A—N2—H2B	120.0	N1—C12—H12	118.4
O2—C1—O1	125.45 (16)	C11—C12—H12	118.4

O2—C1—C2	117.12 (16)	O3—C13—N2	122.54 (16)
O1—C1—C2	117.42 (16)	O3—C13—C10	119.36 (16)
C3—C2—C1	119.50 (16)	N2—C13—C10	118.09 (16)
C3—C2—C7	119.82 (16)	O4—C14—C5	124.77 (19)
C7—C2—C1	120.68 (16)	O4—C14—H14	119.5 (11)
C2—C3—H3	119.9	C5—C14—H14	115.7 (11)
O5—Co1—N1—C8	119.00 (13)	C6—C5—C4—C3	−0.9 (3)
O5^i—Co1—N1—C8	−61.00 (13)	C14—C5—C4—C3	−179.95 (17)
O5—Co1—N1—C12	−54.41 (14)	C4—C5—C14—O4	−170.50 (19)
O5^i—Co1—N1—C12	125.59 (14)	C6—C5—C14—O4	10.4 (3)
O6—Co1—N1—C8	−147.87 (13)	C7—C6—C5—C4	0.6 (3)
O6^i—Co1—N1—C8	32.13 (13)	C7—C6—C5—C14	179.65 (17)
O6—Co1—N1—C12	38.72 (14)	C5—C6—C7—C2	0.1 (3)
O6^i—Co1—N1—C12	−141.28 (14)	C6—C7—C2—C1	178.94 (16)
Co1—N1—C8—C9	−171.09 (13)	C6—C7—C2—C3	−0.5 (3)
C12—N1—C8—C9	2.6 (3)	C10—C9—C8—N1	−0.6 (3)
Co1—N1—C12—C11	171.72 (14)	C8—C9—C10—C11	−2.1 (3)
C8—N1—C12—C11	−2.0 (3)	C8—C9—C10—C13	177.26 (16)
C3—C2—C1—O1	173.53 (16)	C9—C10—C11—C12	2.6 (3)
C3—C2—C1—O2	−5.6 (2)	C13—C10—C11—C12	−176.75 (16)
C7—C2—C1—O1	−5.9 (3)	C9—C10—C13—O3	−174.44 (17)
C7—C2—C1—O2	174.98 (16)	C9—C10—C13—N2	5.0 (3)
C1—C2—C3—C4	−179.23 (16)	C11—C10—C13—O3	4.9 (3)
C7—C2—C3—C4	0.2 (3)	C11—C10—C13—N2	−175.59 (16)
C2—C3—C4—C5	0.5 (3)	C10—C11—C12—N1	−0.6 (3)

Symmetry codes: (i) −x, −y, −z.

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2A⋯O4^{ii}	0.86	2.13	2.9680 (19)	166
N2—H2B⋯O7^{iii}	0.86	2.05	2.8659 (19)	158
O5—H51⋯O1^{iv}	0.916 (18)	1.723 (18)	2.6355 (18)	174.5 (18)
O5—H52⋯O2	0.868 (15)	1.863 (15)	2.7236 (18)	171.1 (18)
O6—H61⋯O1^{v}	0.899 (15)	1.872 (15)	2.7707 (19)	177.3 (11)
O6—H62⋯O2^{vi}	0.87 (2)	1.92 (2)	2.7760 (19)	168 (2)
O7—H71⋯O3^{vii}	0.891 (19)	1.850 (18)	2.7371 (19)	173.7 (18)
O7—H72⋯O4^{ii}	0.936 (15)	1.982 (15)	2.9168 (19)	176.8 (17)
C9—H9⋯O7^{iii}	0.93	2.56	3.458 (2)	161
C12—H12⋯O5^{viii}	0.93	2.45	3.210 (2)	139

Symmetry codes: (ii) x+1, y−1, z+1; (iii) −x, −y, −z+1; (iv) −x, −y+1, −z; (v) x+1, y−1, z; (vi) x, y−1, z; (vii) −x+1, −y, −z+1; (viii) −x+1, −y, −z.

Fig. 1