



Crystal structure of a Co^{II} coordination polymer: *catena*-poly[[μ -aqua-bis(μ -2-methylpropanoato)- κ^2 O:O'; κ^2 O:O-cobalt(II)] monohydrate]

Andrei I. Fischer,^{a*} Vladislav V. Gurzhiy,^{b*} Julia V. Aleksandrova^a and Maria I. Pakina^a

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^aSt Petersburg State Institute of Technology, Moskovsky pr. 26, 190013, St Petersburg, Russian Federation, and ^bInstitute of Earth Sciences, St Petersburg State University, University Emb. 7/9, 199034, St Petersburg, Russian Federation.

*Correspondence e-mail: andreasfischer@mail.ru, vladgeo17@mail.ru

In the title cobalt(II) coordination polymer with isobutyrate ligands, $\{[\text{Co}\{\text{CH}(\text{CH}_3)_2\text{CO}_2\}_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$, the Co²⁺ ion is hexacoordinated in a slightly distorted octahedral coordination environment defined by two O atoms from two bridging water molecules and four O atoms from four bridging carboxylate ligands. The carboxylates adopt two different coordination modes, μ -(κ^2 O:O') and μ -(κ^2 O:O), forming a one-dimensional polymeric chain extending along [010]. The intra-chain cobalt...cobalt separation is 3.2029 (2) Å. The polymeric chains are linked by hydrogen bonds involving the water molecules of solvation, giving a two-dimensional network structure lying parallel to (100).

1. Chemical context

Carboxylate anions still remain a popular choice as bridging ligands because of their ability to form diverse oligo- and polynuclear structures. Oligo- and polynuclear cobalt carboxylates in turn have attracted great attention because of their utilization in homogeneous oxidation catalysis (Gates, 1992; Parshall & Ittel, 1992; Partenheimer, 1995; Ward *et al.*, 2013*a*), and their interesting magnetic properties (Ward *et al.*, 2013*b*; Eremenko *et al.*, 2009). Recently, we have reported on the crystal structures of the hydrated polymeric cobalt(II) propionate (Fischer *et al.*, 2010) and butyrate (Fischer *et al.*, 2011), which were prepared by the reaction of cobalt(II) carbonate hydrate with the corresponding aqueous carboxylic acid. The aim of these studies was to investigate the influence of the steric features of the carboxylate anion on the structure of the resulting compounds. Cobalt(II) carboxylates are of interest for our group as starting materials for the synthesis of mixed-valence cobalt carboxylates (Fischer, Kuznetsov & Belyaev, 2012; Fischer, Kuznetsov, Shchukarev & Belyaev, 2012). In addition, we intend to examine the catalytic activity of the cobalt(II) carboxylates obtained, which will be used for introduction into the sodalite cages of synthetic NaY zeolites, modified by decationation and dealuminizing methods.

As a part of our ongoing studies on these compounds, we describe here synthesis and crystal structure of the title compound, $\{[\text{Co}\{\text{CH}(\text{CH}_3)_2\text{CO}_2\}_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$ (I).

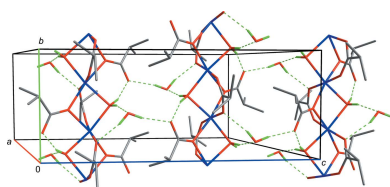


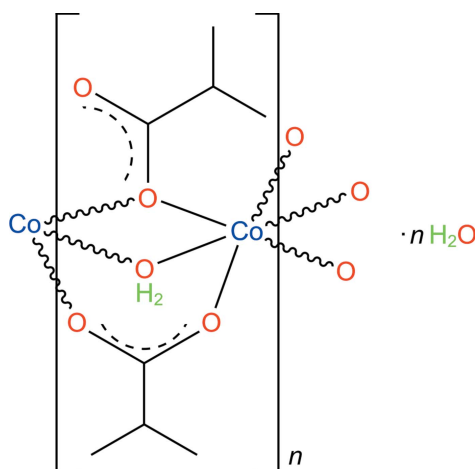
Table 1
Selected geometric parameters (Å, °).

Co1—O1A	2.0449 (6)	Co1—O1B ⁱ	2.1198 (6)
Co1—O2A ⁱ	2.0142 (6)	Co1—O1W	2.1768 (6)
Co1—O1B	2.1100 (6)	Co1—O1W ⁱ	2.1777 (6)
O1A—Co1—O1B	88.13 (3)	O2A ⁱ —Co1—O1W ⁱ	88.33 (3)
O1A—Co1—O1B ⁱ	89.41 (3)	O1B—Co1—O1B ⁱ	170.29 (2)
O1A—Co1—O1W	92.18 (3)	O1B—Co1—O1W	79.22 (2)
O1A—Co1—O1W ⁱ	88.29 (3)	O1B ⁱ —Co1—O1W	91.49 (2)
O2A ⁱ —Co1—O1A	175.30 (3)	O1B—Co1—O1W ⁱ	110.31 (2)
O2A ⁱ —Co1—O1B	89.99 (3)	O1B ⁱ —Co1—O1W ⁱ	78.99 (2)
O2A ⁱ —Co1—O1B ⁱ	93.14 (3)	O1W—Co1—O1W ⁱ	170.46 (2)
O2A ⁱ —Co1—O1W	91.70 (3)		

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$.

2. Structural commentary

The structure of (I) contains one independent Co²⁺ cation coordinated by four O atoms from four bridging isobutyrate ligands and two O atoms from two bridging water molecules (O1W) in a distorted octahedral coordination. A water molecule of solvation (O2W) is also present (Fig. 1). The Co—O bond lengths are in the range 2.0142 (6)–2.1777 (6) Å (Table 1) and the *cis*-angles about the Co²⁺ atom vary in the range 78.99 (3)–110.31 (2)°. This data correlates with the angles and the distances in cobalt(II) acetate dihydrate which has a similar structure (Jiao *et al.*, 2000), as well as with the closely related cobalt(II) propionate dihydrate (Fischer *et al.*, 2010) and cobalt(II) butyrate 1.7-hydrate (Fischer *et al.*, 2011).



The structure of (I) is based on infinite chains with $\infty[\text{Co}(\text{H}_2\text{O})((\text{CH}_3)_2\text{CHCOO})_2]$ composition, extending along [010] (Fig. 2). The Co \cdots Co distance within the chain is 3.2029 (2) Å. The formation of polymeric chains may be a plausible reason for the crystal growth being predominantly along the *b* axis. The bridging carboxylate groups adopt two coordination modes, μ -($\kappa^2\text{O}:\text{O}'$) and μ -($\kappa^2\text{O}:\text{O}$). The C—O bond lengths of the first group (involving O1A and O2A) have close values [1.2755 (10) and 1.2533 (10) Å], whereas those of the second group (involving O1B and O2B) have a more striking difference [1.2878 (9) and 1.2510 (11) Å]. The carboxylate O2B atom of the second group forms an inter-unit

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

<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>
O1W—H1W1 \cdots O2W	0.79 (2)	1.91 (2)	2.6638 (10)	161 (2)
O1W—H1W2 \cdots O2B ⁱ	0.88 (2)	1.79 (2)	2.6206 (9)	158 (2)
O2W—H2W1 \cdots O1A ⁱⁱ	0.86 (1)	2.01 (1)	2.7967 (9)	151 (1)
O2W—H2W2 \cdots O2B ⁱⁱⁱ	0.88 (1)	1.95 (1)	2.8087 (9)	163 (1)
C2B—H2B \cdots O2A ⁱ	0.98	2.47	3.3094 (11)	144

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

hydrogen bond with the bridging water molecule [O1W—H \cdots O2Bⁱ = 2.6206 (9) Å] (Fig. 2, Table 2).

3. Supramolecular features

Metal–organic chain polymers are linked together through the water molecule of solvation (O2W) by a system of hydrogen bonds, forming a sheet structure arranged parallel to (100) (Table 2, Fig. 3). Only weak van der Waals interactions link neighboring sheets in the crystal structure.

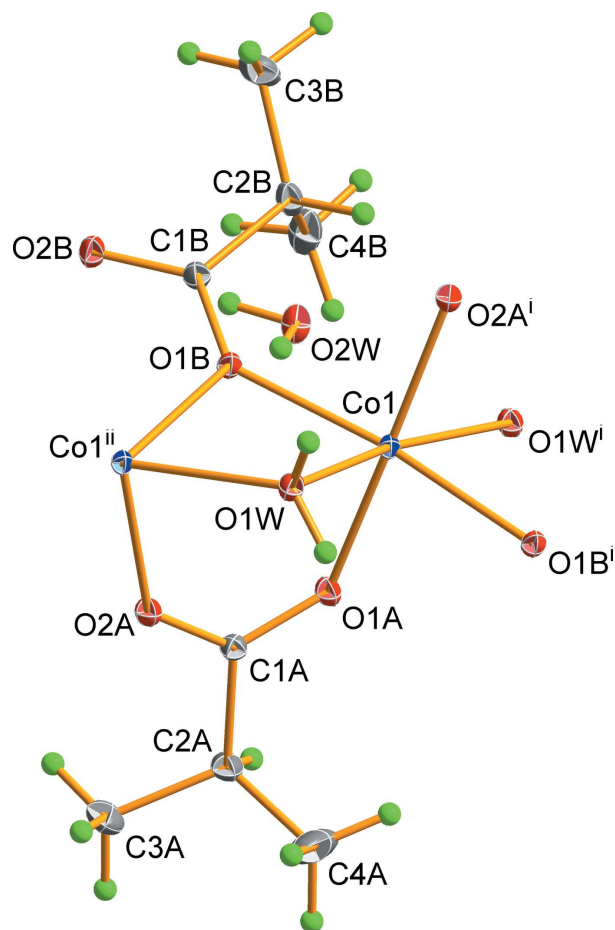


Figure 1
The coordination mode and atom-numbering scheme for (I). Displacement ellipsoids of the non H-atoms are drawn at the 50% probability level, with H atoms shown as spheres of arbitrary radius. [Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.

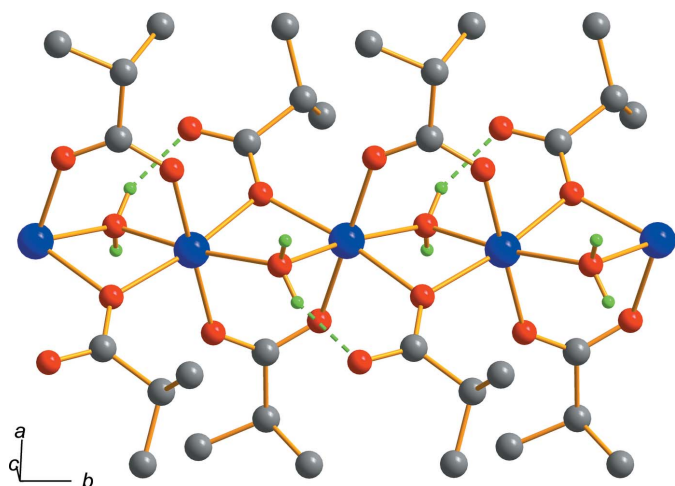


Figure 2
The one-dimensional polymeric structure of (I) extending along [010], with the intramolecular hydrogen bond shown as a dashed line. The carbon-bound H atoms and the water molecule of solvation have been omitted.

4. Database survey

A survey of the Cambridge Structural Database (Groom *et al.*, 2016) reveals only the following related one-dimensional polymeric structures of cobalt(II) carboxylates with composition $\infty[\text{Co}(\text{RCOO})_2(\text{H}_2\text{O})]$: acetate (Jiao *et al.*, 2000), propionate (Fischer *et al.*, 2010) and butyrate (Fischer *et al.*, 2011).

5. Synthesis and crystallization

The title compound was synthesized using a similar procedure as for the synthesis of the analogous carboxylates cobalt(II) propionate dihydrate (Fischer *et al.*, 2010) and cobalt(II) butyrate 1.7-hydrate (Fischer *et al.*, 2011). To a mixture of

Table 3
Experimental details.

Crystal data	
Chemical formula	$[\text{Co}(\text{C}_4\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$
M_r	269.15
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	11.9999 (4), 6.3815 (2), 16.1374 (6)
β (°)	109.540 (2)
V (Å ³)	1164.59 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.48
Crystal size (mm)	0.35 × 0.15 × 0.1
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2014)
$T_{\text{min}}, T_{\text{max}}$	0.304, 0.417
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25308, 5082, 4459
R_{int}	0.070
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.807
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.026, 0.068, 1.03
No. of reflections	5082
No. of parameters	152
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.25, -0.51

Computer programs: APEX2 and SAINT (Bruker, 2014), SHELXS97 (Sheldrick, 2008), SHELXL2012 (Sheldrick, 2015), DIAMOND (Brandenburg, 2012) and OLEX2 (Dolomanov *et al.*, 2009).

isobutyric acid (8.8 g, 100 mmol) and water (100 ml), an excess of fresh cobalt(II) carbonate hexahydrate, $\text{CoCO}_3\cdot 6\text{H}_2\text{O}$, (13.6 g, 60 mmol) was added. The reaction mixture was periodically stirred in an ultrasonic bath at room temperature until the liberation of carbon dioxide ceased. The unreacted $\text{CoCO}_3\cdot 6\text{H}_2\text{O}$ was removed by filtration, and the filtrate was

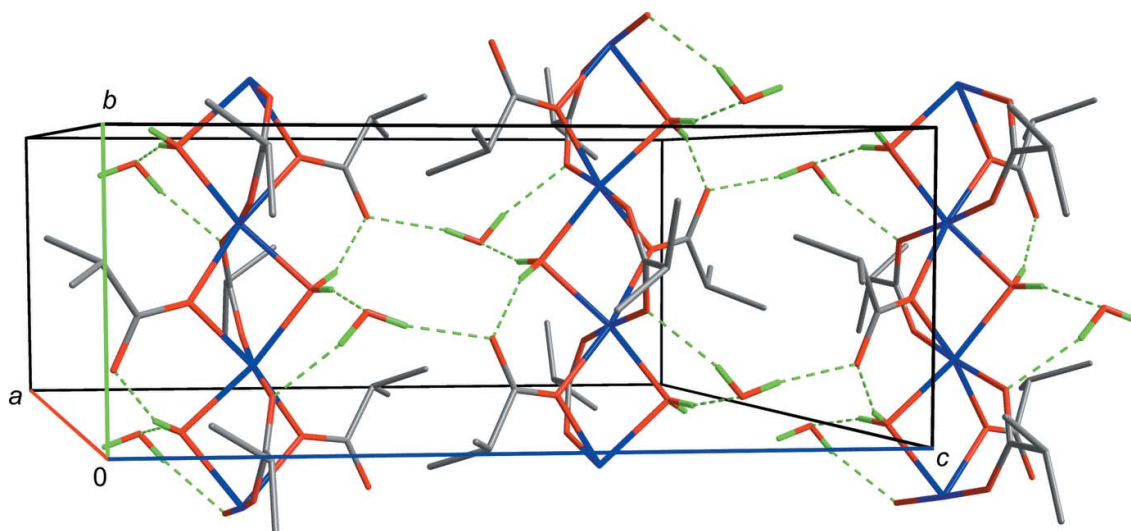


Figure 3
The packing diagram of (I), showing the interactions between the coordination polymer chains. Hydrogen bonds are shown as dashed lines. The carbon-bound H atoms are omitted for clarity.

allowed to stand at room temperature for slow evaporation. Red single crystals of (I) suitable for X-ray diffraction were obtained after several days. The yield was 81%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms of the water molecules were located from difference maps and refined in an isotropic approximation with $U_{\text{iso}}(\text{H})$ set to $1.5U_{\text{eq}}(\text{O})$. Other hydrogen atoms were placed in calculated positions and refined using a riding model with $d(\text{C}-\text{H}) = 0.98 \text{ \AA}$, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the tertiary carbon atoms and $d(\text{C}-\text{H}) = 0.96 \text{ \AA}$, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups.

Acknowledgements

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supporting information

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Crystal structure of a Co^{II} coordination polymer: *catena*-poly[[μ -aqua-bis(μ -2-methylpropanoato)- κ^2 O:O'; κ^2 O:O-cobalt(II)] monohydrate]

Andrei I. Fischer, Vladislav V. Gurzhiy, Julia V. Aleksandrova and Maria I. Pakina

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINTE* (Bruker, 2014); data reduction: *SAINTE* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2012); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

catena-Poly[[μ -aqua-bis(μ -2-methylpropanoato)- κ^2 O:O'; κ^2 O:O-cobalt(II)] monohydrate]

Crystal data

[Co(C₄H₇O₂)₂(H₂O)]·H₂O

$M_r = 269.15$

Monoclinic, $P2_1/c$

$a = 11.9999$ (4) Å

$b = 6.3815$ (2) Å

$c = 16.1374$ (6) Å

$\beta = 109.540$ (2)°

$V = 1164.59$ (7) Å³

$Z = 4$

$F(000) = 564$

$D_x = 1.535$ Mg m⁻³

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

Cell parameters from 9959 reflections

$\theta = 3.5$ – 49.6 °

$\mu = 1.48$ mm⁻¹

$T = 100$ K

Prism, red

$0.35 \times 0.15 \times 0.1$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

$T_{\min} = 0.304$, $T_{\max} = 0.417$

25308 measured reflections

5082 independent reflections

4459 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.070$

$\theta_{\max} = 35.0$ °, $\theta_{\min} = 3.5$ °

$h = -17 \rightarrow 19$

$k = -10 \rightarrow 4$

$l = -26 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.068$

$S = 1.03$

5082 reflections

152 parameters

4 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2]$

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

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

$\Delta\rho_{\max} = 1.25$ e Å⁻³

$\Delta\rho_{\min} = -0.51$ 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.

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	0.49462 (2)	0.68360 (2)	0.24090 (2)	0.00839 (4)
O1A	0.66165 (5)	0.60756 (10)	0.24434 (4)	0.01230 (11)
O2A	0.67317 (6)	0.26293 (11)	0.27311 (4)	0.01275 (11)
O1B	0.43294 (5)	0.41595 (10)	0.16212 (4)	0.01065 (11)
O2B	0.34759 (6)	0.20179 (10)	0.05000 (4)	0.01437 (12)
O1W	0.49903 (6)	0.45171 (10)	0.34088 (4)	0.01116 (11)
H1W1	0.4417 (17)	0.463 (3)	0.3540 (16)	0.017*
H1W2	0.5573 (18)	0.505 (3)	0.3843 (15)	0.017*
O2W	0.29615 (6)	0.39794 (11)	0.37156 (4)	0.01612 (12)
H2W1	0.2869 (13)	0.290 (2)	0.3380 (10)	0.024*
H2W2	0.3027 (13)	0.344 (2)	0.4235 (8)	0.024*
C1A	0.71817 (7)	0.43527 (13)	0.26448 (5)	0.01045 (14)
C2A	0.85034 (8)	0.44468 (14)	0.28101 (6)	0.01530 (15)
H2A	0.8621	0.5188	0.2314	0.018*
C3A	0.90702 (9)	0.2299 (2)	0.28691 (9)	0.0292 (2)
H3A1	0.9021	0.1576	0.3377	0.044*
H3A2	0.9885	0.2457	0.2917	0.044*
H3A3	0.8663	0.1508	0.2350	0.044*
C4A	0.90875 (11)	0.5731 (2)	0.36327 (11)	0.0409 (4)
H4A1	0.8738	0.7102	0.3563	0.061*
H4A2	0.9918	0.5855	0.3726	0.061*
H4A3	0.8976	0.5050	0.4130	0.061*
C1B	0.36124 (7)	0.38036 (14)	0.08390 (5)	0.01115 (14)
C2B	0.29432 (9)	0.56464 (14)	0.03069 (6)	0.01593 (16)
H2B	0.2944	0.6787	0.0714	0.019*
C3B	0.16552 (9)	0.50628 (19)	-0.02026 (7)	0.0238 (2)
H3B1	0.1637	0.3970	-0.0616	0.036*
H3B2	0.1245	0.6271	-0.0512	0.036*
H3B3	0.1278	0.4583	0.0201	0.036*
C4B	0.35856 (10)	0.64054 (17)	-0.03141 (6)	0.02213 (19)
H4B1	0.4358	0.6907	0.0025	0.033*
H4B2	0.3142	0.7519	-0.0676	0.033*
H4B3	0.3660	0.5265	-0.0680	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00921 (6)	0.00625 (7)	0.00890 (5)	0.00009 (3)	0.00197 (4)	-0.00013 (3)
O1A	0.0120 (3)	0.0092 (3)	0.0155 (3)	0.0012 (2)	0.0043 (2)	0.0020 (2)

O2A	0.0116 (3)	0.0097 (3)	0.0164 (3)	0.0002 (2)	0.0040 (2)	0.0016 (2)
O1B	0.0120 (3)	0.0083 (3)	0.0091 (2)	0.00017 (19)	0.00020 (19)	-0.00006 (17)
O2B	0.0182 (3)	0.0100 (3)	0.0114 (3)	0.0011 (2)	0.0003 (2)	-0.00154 (19)
O1W	0.0129 (3)	0.0097 (3)	0.0104 (2)	-0.0009 (2)	0.0032 (2)	-0.00094 (18)
O2W	0.0229 (3)	0.0121 (3)	0.0144 (3)	-0.0006 (2)	0.0076 (2)	-0.0006 (2)
C1A	0.0106 (3)	0.0103 (4)	0.0103 (3)	0.0002 (2)	0.0032 (2)	0.0001 (2)
C2A	0.0105 (3)	0.0139 (4)	0.0217 (4)	-0.0002 (3)	0.0057 (3)	0.0017 (3)
C3A	0.0138 (4)	0.0223 (6)	0.0489 (7)	0.0050 (4)	0.0071 (4)	-0.0045 (5)
C4A	0.0179 (5)	0.0483 (9)	0.0492 (8)	-0.0048 (5)	0.0013 (5)	-0.0285 (6)
C1B	0.0123 (3)	0.0107 (4)	0.0093 (3)	0.0010 (3)	0.0022 (2)	0.0000 (2)
C2B	0.0209 (4)	0.0117 (4)	0.0114 (3)	0.0047 (3)	0.0004 (3)	0.0006 (3)
C3B	0.0187 (4)	0.0263 (6)	0.0210 (4)	0.0078 (4)	-0.0005 (3)	0.0026 (3)
C4B	0.0326 (5)	0.0146 (4)	0.0179 (4)	-0.0008 (4)	0.0067 (4)	0.0039 (3)

Geometric parameters (Å, °)

Co1—O1A	2.0449 (6)	C2A—C4A	1.5176 (16)
Co1—O2A ⁱ	2.0142 (6)	C3A—H3A1	0.9600
Co1—O1B	2.1100 (6)	C3A—H3A2	0.9600
Co1—O1B ⁱ	2.1198 (6)	C3A—H3A3	0.9600
Co1—O1W	2.1768 (6)	C4A—H4A1	0.9600
Co1—O1W ⁱ	2.1777 (6)	C4A—H4A2	0.9600
O1A—C1A	1.2755 (10)	C4A—H4A3	0.9600
O2A—C1A	1.2533 (10)	C1B—C2B	1.5179 (12)
O1B—C1B	1.2878 (9)	C2B—H2B	0.9800
O2B—C1B	1.2510 (11)	C2B—C3B	1.5340 (14)
O1W—H1W1	0.79 (2)	C2B—C4B	1.5329 (14)
O1W—H1W2	0.88 (2)	C3B—H3B1	0.9600
O2W—H2W1	0.861 (12)	C3B—H3B2	0.9600
O2W—H2W2	0.884 (11)	C3B—H3B3	0.9600
C1A—C2A	1.5191 (12)	C4B—H4B1	0.9600
C2A—H2A	0.9800	C4B—H4B2	0.9600
C2A—C3A	1.5187 (15)	C4B—H4B3	0.9600
O1A—Co1—O1B	88.13 (3)	C4A—C2A—C3A	111.50 (9)
O1A—Co1—O1B ⁱ	89.41 (3)	C2A—C3A—H3A1	109.5
O1A—Co1—O1W	92.18 (3)	C2A—C3A—H3A2	109.5
O1A—Co1—O1W ⁱ	88.29 (3)	C2A—C3A—H3A3	109.5
O2A ⁱ —Co1—O1A	175.30 (3)	H3A1—C3A—H3A2	109.5
O2A ⁱ —Co1—O1B	89.99 (3)	H3A1—C3A—H3A3	109.5
O2A ⁱ —Co1—O1B ⁱ	93.14 (3)	H3A2—C3A—H3A3	109.5
O2A ⁱ —Co1—O1W	91.70 (3)	C2A—C4A—H4A1	109.5
O2A ⁱ —Co1—O1W ⁱ	88.33 (3)	C2A—C4A—H4A2	109.5
O1B—Co1—O1B ⁱ	170.29 (2)	C2A—C4A—H4A3	109.5
O1B—Co1—O1W	79.22 (2)	H4A1—C4A—H4A2	109.5
O1B ⁱ —Co1—O1W	91.49 (2)	H4A1—C4A—H4A3	109.5
O1B—Co1—O1W ⁱ	110.31 (2)	H4A2—C4A—H4A3	109.5
O1B ⁱ —Co1—O1W ⁱ	78.99 (2)	O1B—C1B—C2B	118.13 (8)

O1W—Co1—O1W ⁱ	170.46 (2)	O2B—C1B—O1B	122.42 (8)
C1A—O1A—Co1	130.11 (6)	O2B—C1B—C2B	119.42 (7)
C1A—O2A—Co1 ⁱⁱ	131.28 (6)	C1B—C2B—H2B	108.3
Co1—O1B—Co1 ⁱⁱ	98.44 (2)	C1B—C2B—C3B	111.27 (8)
C1B—O1B—Co1	135.89 (6)	C1B—C2B—C4B	109.15 (8)
C1B—O1B—Co1 ⁱⁱ	125.09 (6)	C3B—C2B—H2B	108.3
Co1—O1W—Co1 ⁱⁱ	94.70 (2)	C4B—C2B—H2B	108.3
Co1—O1W—H1W1	109.1 (16)	C4B—C2B—C3B	111.30 (8)
Co1 ⁱⁱ —O1W—H1W1	116.6 (14)	C2B—C3B—H3B1	109.5
Co1—O1W—H1W2	98.2 (15)	C2B—C3B—H3B2	109.5
Co1 ⁱⁱ —O1W—H1W2	127.6 (14)	C2B—C3B—H3B3	109.5
H1W1—O1W—H1W2	106 (2)	H3B1—C3B—H3B2	109.5
H2W1—O2W—H2W2	103.8 (14)	H3B1—C3B—H3B3	109.5
O2A—C1A—O1A	124.94 (8)	H3B2—C3B—H3B3	109.5
O2A—C1A—C2A	118.59 (7)	C2B—C4B—H4B1	109.5
O1A—C1A—C2A	116.46 (7)	C2B—C4B—H4B2	109.5
C1A—C2A—H2A	107.6	C2B—C4B—H4B3	109.5
C3A—C2A—C1A	113.25 (8)	H4B1—C4B—H4B2	109.5
C3A—C2A—H2A	107.6	H4B1—C4B—H4B3	109.5
C4A—C2A—C1A	108.94 (8)	H4B2—C4B—H4B3	109.5
C4A—C2A—H2A	107.6		
Co1—O1A—C1A—C2A	-166.13 (6)	Co1 ⁱⁱ —O1B—C1B—O2B	-16.84 (12)
Co1—O1A—C1A—O2A	12.38 (12)	Co1—O1B—C1B—C2B	-4.15 (12)
O1A—C1A—C2A—C3A	-168.74 (8)	Co1 ⁱⁱ —O1B—C1B—C2B	165.09 (6)
O1A—C1A—C2A—C4A	66.57 (12)	O1B—C1B—C2B—C3B	-138.98 (8)
O2A—C1A—C2A—C3A	12.65 (12)	O1B—C1B—C2B—C4B	97.80 (9)
O2A—C1A—C2A—C4A	-112.03 (11)	O2B—C1B—C2B—C3B	42.89 (11)
Co1—O1B—C1B—O2B	173.93 (6)	O2B—C1B—C2B—C4B	-80.33 (10)

Symmetry codes: (i) $-x+1, y+1/2, -z+1/2$; (ii) $-x+1, y-1/2, -z+1/2$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W1 \cdots O2W	0.79 (2)	1.91 (2)	2.6638 (10)	161 (2)
O1W—H1W2 \cdots O2B ⁱ	0.88 (2)	1.79 (2)	2.6206 (9)	158 (2)
O2W—H2W1 \cdots O1A ⁱⁱ	0.86 (1)	2.01 (1)	2.7967 (9)	151 (1)
O2W—H2W2 \cdots O2B ⁱⁱⁱ	0.88 (1)	1.95 (1)	2.8087 (9)	163 (1)
C2B—H2B \cdots O2A ⁱ	0.98	2.47	3.3094 (11)	144

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