

Racemic dipotassium di- μ_2 -hydroxido-bis[[*N,N*-bis(carboxylatomethyl)leucinato- $\kappa^4 N, O, O', O''$]]cobaltate(III)] tetrahydrate

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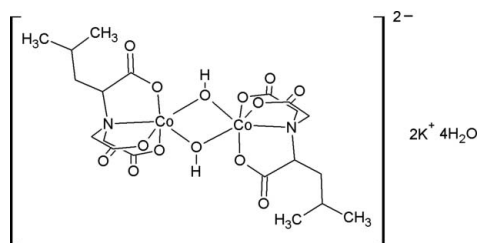
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; H-atom completeness 78%; disorder in main residue; R factor = 0.054; wR factor = 0.133; data-to-parameter ratio = 15.0.

The racemic title compound, $\text{K}_2[\text{Co}_2(\text{C}_{10}\text{H}_{13}\text{NO}_6)_2(\text{OH})_2] \cdot 4\text{H}_2\text{O}$, exhibits a slightly distorted octahedral coordination of the Co atoms, possibly because of constraints imposed by the tetradentate ligand. The ten-coordinate potassium cation provides a link between the ligating anions of the dinuclear dianion *via* the carbonyl O atoms of the *N,N*-bis(carboxylatomethyl)leucinate ligands, forming a polymeric three-dimensional network. The complex crystallizes in the orthorhombic space group, *Cmca*, resulting in Co dimers situated around special positions in the unit cell, which leads to a 50% disorder of the bridging hydroxido H atoms and the isopropyl substituents.

Related literature

For crystal structures of related compounds, see: Bocarsley *et al.* (1990); Choi *et al.* (2003); Kato *et al.* (2006); Kumita *et al.* (1998); Novitchi *et al.* (2005); Skrzypczak-Jankun *et al.* (1994); Visser *et al.* (1997, 2001, 2005); Whitlow (1972). For the ring notation, see: Weakliem & Hoard (1959). For solution studies and kinetics, see: Visser *et al.* (2002, 2003, 2006).



Experimental

Crystal data

$\text{K}_2[\text{Co}_2(\text{C}_{10}\text{H}_{13}\text{NO}_6)_2(\text{OH})_2]$
 $M_r = 788.56$
 Orthorhombic, *Cmca*
 $a = 12.968$ (5) Å
 $b = 25.868$ (5) Å
 $c = 9.240$ (5) Å

$V = 3100$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.42$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.19 \times 0.02$ mm

Data collection

Bruker Kappa APEXII diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
 $T_{\min} = 0.722$, $T_{\max} = 0.969$

8534 measured reflections
 2015 independent reflections
 1700 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.133$
 $S = 1.24$
 2015 reflections
 134 parameters
 33 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.63$ e Å⁻³
 $\Delta\rho_{\min} = -0.66$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co—O1	1.897 (4)	Co—O2	1.913 (3)
Co—O5	1.900 (4)	Co—O2 ⁱⁱ	1.913 (3)
Co—O5 ⁱ	1.909 (4)	Co—N	1.930 (4)
O1—Co—O5	173.32 (16)	O5 ⁱ —Co—O2 ⁱⁱ	94.12 (8)
O1—Co—O5 ⁱ	92.31 (17)	O2—Co—O2 ⁱⁱ	171.76 (16)
O5—Co—O5 ⁱ	81.01 (18)	O1—Co—N	87.65 (18)
O1—Co—O2	90.02 (9)	O5—Co—N	99.03 (18)
O5—Co—O2	90.46 (9)	O5 ⁱ —Co—N	179.96 (19)
O5 ⁱ —Co—O2	94.12 (8)	O2—Co—N	85.88 (8)
O1—Co—O2 ⁱⁱ	90.02 (9)	O2 ⁱⁱ —Co—N	85.88 (8)
O5—Co—O2 ⁱⁱ	90.46 (9)		

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2364).

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Acta Cryst. (2007). E63, m2998-m2999 [doi:10.1107/S1600536807056437]

Racemic dipotassium di- μ_2 -hydroxido-bis{[*N,N*-bis(carboxylatomethyl)leucinato- κ^4N,O,O',O'']}cobaltate(III)} tetrahydrate

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Comment

Tripod type ligands like nitrilotriacetic acid (nta) and the very similar *N,N*-bis(carboxymethyl) *d,l*-leucinate (*d,l*-lda) are of special interest to us in terms of its applicability as chelation agents of heavy metal ions in industrial effluents (Novitchi *et al.*, 2005; Choi *et al.*, 2003). Also, the fact that these ligands imitate simple biological systems make the investigation into the coordination chemistry and kinetic behaviour of complexes with metal ions like chromium(III) and cobalt(III) quite interesting (Bocarsley *et al.*, 1990; Visser *et al.*, 2002; Visser *et al.*, 2006).

The title compound (I, see Fig. 1) crystallizes in the orthorhombic space group *Cmca* ($Z=8$), resulting in Co-dimers situated around special positions in the unit cell. The two cobalt centres are octahedrally surrounded by the nitrogen and three carboxylate O atoms of the lda ligand plus the two bridging hydroxo oxygen atoms. The lda ligand forms three glycinate rings around the central metal ion. These rings can be classified into one *R* ring, Co—N—C(2)—C(1)—O(1) and two *G* rings, Co—N—C(4)—C(3)—O(2) and Co—N—C(4)^{*i*}—C(3)^{*i*}—O(2)^{*i*} according to the notations used by Weakliem *et al.* (1959) (Symmetry code *i* = $-x,y,z$).

The octahedral environment around the Co(III) atoms are substantially distorted. The Co—O bond distances vary between 1.897 (4) and 1.913 (3) Å, while the Co—N bond distance is 1.930 (4) Å. All the N—Co—O bond angles deviate from 90° and range between 85.88 (8) and 99.03 (18)°.

The Co—N and Co—O bond distances correspond well with that found for [Co(nta)(μ -OH)]₂²⁻ [Visser *et al.*, 1997]. The N—C, C—C and C—O bonding distances within the lda ligand correspond well with those obtained for Ca(nta)·2H₂O (Whitlow, 1972) and Hnta (Skrzypczak-Jankun *et al.*, 1994). The nitrogen tetrahedron is slightly distorted with angles varying between 111.3 (3) and 114.9 (5)°.

Each potassium cation interacts with ten oxygen atoms (two water molecules and eight carboxylate O atoms from three different anions), serving as a link between the anions and generating a polymeric network. The K⁺ to oxygen interatomic distances vary between 2.827 (3) and 3.077 (4) Å. Further links between the anions are provided by an extensive network of hydrogen bonds (see Table 2).

Experimental

K₂[Co(*d,l*-lda)(μ -OH)]₂·2H₂O, was prepared by the method similar to that used for Cs₂[Co(nta)(μ -OH)]₂·2H₂O [Visser *et al.*, 1997]. CoCl₂·6H₂O (2 g, 0.008 mol) and *N,N*-bis(carboxymethyl) *d,l*-leucinate (2.08 g, 0.008 mol) was added to a KHCO₃ solution (5 g, 0.05 mol) and heated on a water bath. The pH of the solution was adjusted to 6 – 7 and this solution was placed on an ice bath. H₂O₂ (1 cm³, 30%) was added to the solution and after a few hours a bluish violate precipitate separated out from the solution. The precipitate was filtered and dried. Re-crystallization was carried out in water

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and blue/purple crystals, suitable for X-ray crystallography, were obtained after a few days. yield: 63.9%. IR $\nu(\text{COOH})$ 1625 cm^{-1} . UV-Vis λ_{max} 304, 400, 565 nm. ^1H NMR (D_2O , p.p.m.): 0.95 (d, 6H), 1.65 (m, 1H), 1.90 (m, 2H), 3.56 (d, 1H), 3.85 (d, 1H), 3.82(d, 1H), 4.44 (d, 1H), 4.44 (t, 1H).

Refinement

The methine, methylene and methyl H atoms were placed in geometrically idealized positions ($\text{C}-\text{H} = 0.93-0.98$) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methine and methylene, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl respectively. Methyl torsion angles were refined from electron density. Bridging hydroxo H atoms were located from a Fourier difference map and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. These show a 50% disorder due to molecules being situated on special positions in the unit cell. The isopropyl substituents are also 50% disordered for the same reason and also show high thermal vibrations on the periphery. Possible hydrogen coordinates from the Fourier difference map could not be refined satisfactory for the water solvate.

Figures

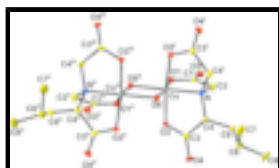


Fig. 1. View of (I) (50% probability displacement ellipsoids). Hydrogen atoms have been omitted for clarity. Atoms labels containing superscripts indicates atoms generated by symmetry (symmetry codes i = $-x, y, z$; ii = $x, -y, 1 - z$; iii = $-x, -y, 1 - z$)

dipotassium di- μ_2 -hydroxido-bis{[*N,N*-bis(carboxylatomethyl)leucinato- $\kappa^4\text{N},\text{O},\text{O}',\text{O}''$]}cobaltate(III)} tetrahydrate

Crystal data

$\text{K}_2[\text{Co}_2(\text{C}_{10}\text{H}_{13}\text{NO}_6)_2(\text{OH})_2]$

$M_r = 788.56$

Orthorhombic, *Cmca*

Hall symbol: $-C\ 2bc\ 2$

$a = 12.968\ (5)\ \text{\AA}$

$b = 25.868\ (5)\ \text{\AA}$

$c = 9.240\ (5)\ \text{\AA}$

$V = 3100\ (2)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1624$

$D_x = 1.69\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1747 reflections

$\theta = 2.7-28.1^\circ$

$\mu = 1.42\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Plate, purple

$0.25 \times 0.19 \times 0.02\ \text{mm}$

Data collection

Bruker Kappa APEXII
diffractometer

Monochromator: graphite

Detector resolution: $512\ \text{pixels mm}^{-1}$

$T = 100(2)\ \text{K}$

2015 independent reflections

1700 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.060$

$\theta_{\text{max}} = 28.4^\circ$

φ and ω scans	$\theta_{\min} = 2.8^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -15 \rightarrow 17$
$T_{\min} = 0.722$, $T_{\max} = 0.969$	$k = -30 \rightarrow 34$
8534 measured reflections	$l = -10 \rightarrow 12$

Refinement

Refinement on F^2	33 restraints
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2 + 25.1765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.24$	$\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$
2015 reflections	$\Delta\rho_{\min} = -0.66 \text{ e } \text{\AA}^{-3}$
134 parameters	Extinction correction: none

Special details

Experimental. The intensity data was collected on a Bruker X8 Apex II 4 K Kappa CCD diffractometer using an exposure time of 20 s/frame. A total of 620 frames were collected with a frame width of 0.5° covering up to $\theta = 28.4^\circ$ with 98.8% completeness accomplished.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co	0	0.03898 (3)	0.61246 (8)	0.00824 (19)	
C1	0	0.0787 (2)	0.8831 (6)	0.0122 (10)	
C2	0	0.1258 (2)	0.7900 (6)	0.0165 (11)	
H2A	-0.0604	0.1464	0.8123	0.02*	0.5
H2B	0.0604	0.1464	0.8123	0.02*	0.5
C3	-0.1807 (3)	0.09039 (14)	0.5868 (4)	0.0129 (8)	
C4	-0.0971 (3)	0.13099 (14)	0.5611 (5)	0.0174 (8)	
H4	-0.0817	0.1271	0.4579	0.021*	
C5	-0.1206 (6)	0.1870 (3)	0.5748 (10)	0.0187 (14)	0.5
H5A	-0.0584	0.2047	0.6058	0.022*	0.5
H5B	-0.1717	0.1914	0.6505	0.022*	0.5
C6	-0.1607 (8)	0.2135 (4)	0.4365 (12)	0.0320 (18)	0.5
H6	-0.2166	0.1927	0.395	0.038*	0.5
C7	-0.0754 (10)	0.2203 (4)	0.3234 (14)	0.047 (3)	0.5
H7A	-0.0226	0.2425	0.3615	0.07*	0.5
H7B	-0.1039	0.2355	0.2375	0.07*	0.5

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H7C	-0.0461	0.1872	0.3004	0.07*	0.5
C8	-0.2027 (10)	0.2676 (4)	0.4777 (17)	0.054 (3)	0.5
H8A	-0.2632	0.2638	0.5365	0.081*	0.5
H8B	-0.2198	0.2863	0.3913	0.081*	0.5
H8C	-0.151	0.2862	0.5307	0.081*	0.5
N	0	0.11323 (16)	0.6325 (5)	0.0097 (9)	
O1	0	0.03494 (14)	0.8175 (4)	0.0113 (8)	
O2	-0.1472 (2)	0.04429 (10)	0.6132 (3)	0.0124 (5)	
O3	0	0.08247 (15)	1.0160 (4)	0.0156 (8)	
O4	-0.2731 (2)	0.10165 (11)	0.5758 (3)	0.0187 (6)	
O5	0	0.03447 (14)	0.4072 (4)	0.0129 (8)	
O6	-0.3530 (2)	-0.08192 (14)	0.7397 (4)	0.0329 (8)	
K	-0.33220 (9)	0	0.5	0.0170 (3)	
H5	-0.057 (4)	0.043 (4)	0.373 (10)	0.02*	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0076 (4)	0.0083 (3)	0.0088 (4)	0	0	0.0003 (3)
C1	0.005 (2)	0.017 (2)	0.015 (3)	0	0	-0.002 (2)
C2	0.023 (3)	0.013 (3)	0.013 (3)	0	0	-0.002 (2)
C3	0.0126 (19)	0.0149 (17)	0.0113 (18)	-0.0007 (14)	-0.0036 (15)	-0.0022 (13)
C4	0.014 (2)	0.0114 (16)	0.027 (2)	0.0023 (13)	-0.0090 (17)	0.0012 (15)
C5	0.011 (3)	0.014 (2)	0.031 (3)	0.005 (2)	-0.006 (3)	-0.004 (3)
C6	0.025 (4)	0.024 (3)	0.048 (4)	0.010 (3)	-0.008 (3)	0.013 (3)
C7	0.055 (7)	0.031 (5)	0.054 (6)	0.006 (5)	0.008 (5)	0.025 (5)
C8	0.053 (7)	0.025 (4)	0.083 (9)	0.021 (4)	0.001 (6)	0.019 (5)
N	0.007 (2)	0.0090 (19)	0.013 (2)	0	0	0.0007 (16)
O1	0.0124 (19)	0.0118 (17)	0.0096 (19)	0	0	0.0002 (14)
O2	0.0092 (13)	0.0119 (12)	0.0160 (14)	-0.0005 (9)	-0.0022 (11)	-0.0003 (11)
O3	0.013 (2)	0.023 (2)	0.0110 (19)	0	0	-0.0016 (16)
O4	0.0105 (14)	0.0187 (14)	0.0268 (17)	0.0053 (10)	-0.0044 (13)	-0.0020 (12)
O5	0.015 (2)	0.0105 (17)	0.013 (2)	0	0	0.0004 (14)
O6	0.0193 (17)	0.055 (2)	0.0243 (18)	0.0144 (15)	-0.0040 (14)	-0.0127 (16)
K	0.0101 (6)	0.0144 (5)	0.0265 (7)	0	0	-0.0036 (5)

Geometric parameters (\AA , $^\circ$)

Co—O1	1.897 (4)	C4—N	1.494 (4)
Co—O5	1.900 (4)	C4—H4	0.98
Co—O5 ⁱ	1.909 (4)	C5—C6	1.540 (13)
Co—O2	1.913 (3)	C5—H5A	0.97
Co—O2 ⁱⁱ	1.913 (3)	C5—H5B	0.97
Co—N	1.930 (4)	C6—C7	1.532 (16)
Co—Co ⁱ	2.8959 (16)	C6—C8	1.550 (14)
C1—O3	1.232 (7)	C6—H6	0.98
C1—O1	1.283 (6)	C7—H7A	0.96
C1—C2	1.491 (8)	C7—H7B	0.96

C2—N	1.491 (7)	C7—H7C	0.96
C2—H2A	0.97	C8—H8A	0.96
C2—H2B	0.97	C8—H8B	0.96
C3—O4	1.237 (5)	C8—H8C	0.96
C3—O2	1.293 (4)	N—C4 ⁱⁱ	1.494 (4)
C3—C4	1.528 (5)	O5—Co ⁱ	1.909 (4)
C4—C5	1.485 (8)	O5—H5	0.83 (2)
O1—Co—O5	173.32 (16)	N—C4—H4	103
O1—Co—O5 ⁱ	92.31 (17)	C3—C4—H4	103
O5—Co—O5 ⁱ	81.01 (18)	C4—C5—C6	115.6 (7)
O1—Co—O2	90.02 (9)	C4—C5—H5A	108.4
O5—Co—O2	90.46 (9)	C6—C5—H5A	108.4
O5 ⁱ —Co—O2	94.12 (8)	C4—C5—H5B	108.4
O1—Co—O2 ⁱⁱ	90.02 (9)	C6—C5—H5B	108.4
O5—Co—O2 ⁱⁱ	90.46 (9)	H5A—C5—H5B	107.4
O5 ⁱ —Co—O2 ⁱⁱ	94.12 (8)	C7—C6—C5	111.9 (8)
O2—Co—O2 ⁱⁱ	171.76 (16)	C7—C6—C8	108.5 (9)
O1—Co—N	87.65 (18)	C5—C6—C8	108.5 (9)
O5—Co—N	99.03 (18)	C7—C6—H6	109.3
O5 ⁱ —Co—N	179.96 (19)	C5—C6—H6	109.3
O2—Co—N	85.88 (8)	C8—C6—H6	109.3
O2 ⁱⁱ —Co—N	85.88 (8)	C6—C7—H7A	109.5
O1—Co—Co ⁱ	132.70 (12)	C6—C7—H7B	109.5
O5—Co—Co ⁱ	40.62 (11)	H7A—C7—H7B	109.5
O5 ⁱ —Co—Co ⁱ	40.39 (12)	C6—C7—H7C	109.5
O2—Co—Co ⁱ	93.01 (8)	H7A—C7—H7C	109.5
O2 ⁱⁱ —Co—Co ⁱ	93.01 (8)	H7B—C7—H7C	109.5
N—Co—Co ⁱ	139.65 (14)	C6—C8—H8A	109.5
O3—C1—O1	122.8 (5)	C6—C8—H8B	109.5
O3—C1—C2	120.6 (5)	H8A—C8—H8B	109.5
O1—C1—C2	116.6 (5)	C6—C8—H8C	109.5
N—C2—C1	112.7 (4)	H8A—C8—H8C	109.5
N—C2—H2A	109.1	H8B—C8—H8C	109.5
C1—C2—H2A	109.1	C2—N—C4	111.3 (3)
N—C2—H2B	109.1	C2—N—C4 ⁱⁱ	111.3 (3)
C1—C2—H2B	109.1	C4—N—C4 ⁱⁱ	114.9 (5)
H2A—C2—H2B	107.8	C2—N—Co	108.1 (3)
O4—C3—O2	124.0 (4)	C4—N—Co	105.3 (2)
O4—C3—C4	120.8 (3)	C4 ⁱⁱ —N—Co	105.3 (2)
O2—C3—C4	115.1 (3)	C1—O1—Co	115.0 (3)
C5—C4—N	115.8 (5)	C3—O2—Co	113.7 (2)
C5—C4—C3	120.8 (5)	Co—O5—Co ⁱ	98.99 (18)
N—C4—C3	108.6 (3)	Co—O5—H5	111 (7)
C5—C4—H4	103	Co ⁱ —O5—H5	103 (7)

supplementary materials

O3—C1—C2—N	180.000 (2)	O2—Co—N—C4	-28.9 (3)
O1—C1—C2—N	0.000 (2)	O2 ⁱⁱ —Co—N—C4	150.7 (3)
O4—C3—C4—C5	22.2 (7)	Co ⁱ —Co—N—C4	60.9 (3)
O2—C3—C4—C5	-160.9 (5)	O1—Co—N—C4 ⁱⁱ	119.1 (3)
O4—C3—C4—N	159.4 (4)	O5—Co—N—C4 ⁱⁱ	-60.9 (3)
O2—C3—C4—N	-23.7 (5)	O2—Co—N—C4 ⁱⁱ	-150.7 (3)
N—C4—C5—C6	137.6 (7)	O2 ⁱⁱ —Co—N—C4 ⁱⁱ	28.9 (3)
C3—C4—C5—C6	-88.1 (8)	Co ⁱ —Co—N—C4 ⁱⁱ	-60.9 (3)
C4—C5—C6—C7	-72.3 (10)	O3—C1—O1—Co	180.0000 (10)
C4—C5—C6—C8	168.1 (8)	C2—C1—O1—Co	0.0000 (10)
C1—C2—N—C4	115.2 (3)	O2—Co—O1—C1	-85.88 (8)
C1—C2—N—C4 ⁱⁱ	-115.2 (3)	O2 ⁱⁱ —Co—O1—C1	85.88 (8)
C1—C2—N—Co	0.0000 (10)	N—Co—O1—C1	0.0000 (10)
C5—C4—N—C2	57.3 (6)	Co ⁱ —Co—O1—C1	180.0000 (10)
C3—C4—N—C2	-82.3 (4)	O4—C3—O2—Co	176.6 (3)
C5—C4—N—C4 ⁱⁱ	-70.5 (7)	C4—C3—O2—Co	-0.2 (4)
C3—C4—N—C4 ⁱⁱ	149.9 (3)	O1—Co—O2—C3	105.1 (3)
C5—C4—N—Co	174.2 (5)	O5—Co—O2—C3	-81.5 (3)
C3—C4—N—Co	34.5 (4)	O5 ⁱ —Co—O2—C3	-162.5 (3)
O1—Co—N—C2	0	N—Co—O2—C3	17.5 (3)
O5—Co—N—C2	180	Co ⁱ —Co—O2—C3	-122.1 (3)
O2—Co—N—C2	90.19 (9)	O5 ⁱ —Co—O5—Co ⁱ	0
O2 ⁱⁱ —Co—N—C2	-90.19 (9)	O2—Co—O5—Co ⁱ	-94.10 (8)
Co ⁱ —Co—N—C2	180.0000 (10)	O2 ⁱⁱ —Co—O5—Co ⁱ	94.10 (8)
O1—Co—N—C4	-119.1 (3)	N—Co—O5—Co ⁱ	180
O5—Co—N—C4	60.9 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5 ⁱⁱⁱ —O6 ⁱⁱⁱ	0.83 (2)	1.98 (5)	2.745 (4)	153 (9)
C4—H4 ⁱⁱⁱ —O6 ⁱⁱⁱ	0.98	2.48	3.294 (6)	140

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

Fig. 1

