Crystal structure of poly[diaqua(μ-2-carboxy-acetato-κ³O,O′:O″)(2-carboxyacetato-κO)di-μ-chlorido-dicobalt(II)]

Yasmina Bouaoud,[a] Zouaoui Setifi,[a,b]* Andrii Buvailo,[c,d]* Vadim A. Potaskalov,[e] Hocine Merazig[a] and Georges Dénés[f]

[a]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale (CHEMS), Université Constantine 1, Constantine 25000, Algeria, [b]Laboratoire de Chimie, Ingénierie Moléculaire et Nanostructures (LCIMN), Université Ferhat Abbas Sétif 1, Sétif 19000, Algeria, [c]National Taras Shevchenko University of Kyiv, Department of Chemistry, Volodymyrska str. 64, 01601 Kiev, Ukraine, [d]SciMax LLC, 2 Marshala Yakubovskogo str. 03191, Kyiv, Ukraine, [e]Department of General and Inorganic Chemistry, National Technical University of Ukraine, 'Kyiv Polytechnic Institute', 37 Prospect Peremogy, 03056 Kiev, Ukraine, and [f]Laboratory of Solid State Chemistry and Mössbauer Spectroscopy, Laboratories for Inorganic Materials, Department of Chemistry and Biochemistry, Concordia University, Montréal, Québec, H3G 1M8, Canada. *Correspondence e-mail: setifi_zouaoui@yahoo.fr, futureintentions@gmail.com

The asymmetric unit of the title polymer, $[Co_2(C_3H_3O_4)_2Cl_2(H_2O)_2]_n$, comprises one Co^{II} atom, one water molecule, one singly deprotonated malonic acid molecule ($HMal^-$; systematic name 2-carboxyacetate) and one Cl^- anion. The Co^{II} atom is octahedrally coordinated by the O atom of a water molecule, by one terminally bound carboxylate O atom of an $HMal^-$ anion and by two O atoms of a chelating $HMal^-$ anion, as well as by two Cl^- anions. The Cl^- anions bridge two Co^{II} atoms, forming a centrosymmetric Co_2Cl_2 core. Each malonate ligand is involved in the formation of six-membered chelate rings involving one Co^{II} atom of the dinuclear unit and at the same time is coordinating to another Co^{II} atom of a neighbouring dinuclear unit in a bridging mode. The combination of chelating and bridging coordination modes leads to the formation of a two-dimensional coordination polymer extending parallel to (001). Within a layer, $O-H_{water}\cdots Cl$ and $O-H_{water}\cdots O$ hydrogen bonds are present. Adjacent layers are linked through $O-H\cdots O=C$ hydrogen bonds involving the carboxylic acid OH and carbonyl groups.

1. Chemical context

Complexes with paramagnetic metal ions and extended structures are interesting due to their potential applications in molecular magnetism (Moroz *et al.*, 2012; Pavlishchuk *et al.*, 2010, 2011; Yuste *et al.*, 2009). Malonic acid exhibits both chelating and bridging modes of coordination and is an efficient ligand for achieving two- or three-dimensional polymeric structures (Delgado *et al.*, 2004). In the present communication we report on the structure of a two-dimensional coordination polymer, $[Co(C_3H_3O_4)Cl(H_2O)]_n$, containing both chelating and bridging functions of singly deprotonated malonic acid ligands.

2. Structural commentary

The structure of the title compound is characterized by the presence of a two-dimensional coordination polymer extending parallel to (001). The monomeric fragment can be described as being composed of a centrosymmetric binuclear Co_2Cl_4 motif with the Co^{II} atoms having an overall distorted octahedral environment. The two octahedra are fused
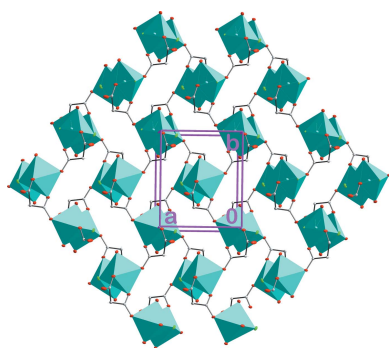
together *via* two bridging Cl atoms with Co—Cl bond lengths of 2.4312 (12) and 2.4657 (16) Å.
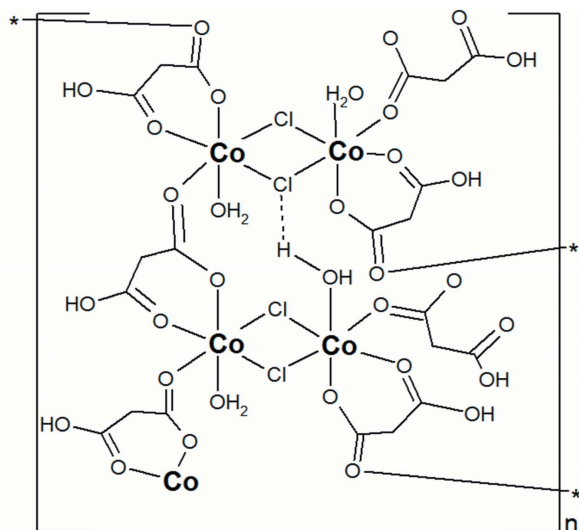
In the octahedron, the Cl⁻ atoms occupy equatorial positions, the other two equatorial positions being defined by the carboxylate O atom of a bridging hydrogenmalonate anion (HMal⁻) and one O atom of a chelating HMal⁻ anion, while
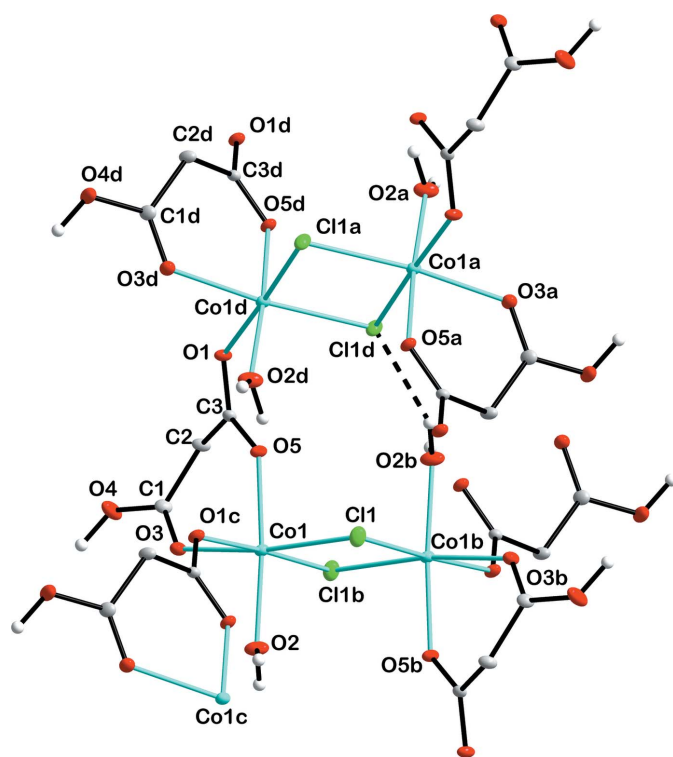

Figure 1
A fragment of the title coordination polymer, showing the atom labelling. All H atoms, except those of hydroxy groups, have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level. The intralayer O—H⋯Cl hydrogen bonds are shown as dashed lines. [Symmetry codes: (a) $\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$; (b) $1 - x, 1 - y, 1 - z$; (c) $\frac{3}{2} - x, -\frac{1}{2} + y, z$; (d) $\frac{3}{2} - x, \frac{1}{2} + y, z$.]

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H1$O2$⋯O5[i]	0.93	1.94	2.689 (4)	136
O2—H2$O2$⋯Cl1[ii]	0.92	2.32	3.135 (3)	147
O4—H1$O4$⋯O1[iii]	0.97	1.67	2.629 (4)	169

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

one water O atom and the other O atom of the chelating HMal⁻ anion are in axial positions (Fig. 1). The corresponding Co—O$_{\text{malonate}}$ bond lengths range from 2.051 (3) to 2.165 (3) Å which is similar to other structures containing this ligand in chelating and bridging modes (Delgado *et al.*, 2004). The Co—O$_{\text{water}}$ bond has a length of 2.046 (3) Å. The C—O bond lengths in the carboxylic group differ significantly [1.225 (2) and 1.306 (4) Å] while those in the carboxylate group [1.258 (4) and 1.267 (4) Å] are more or less the same, which is typical for this functional group (Wörl *et al.*, 2005a,b).

3. Supramolecular features

The distribution of the dinuclear units within a coordination layer follows a chess-like pattern whereby each dinuclear coordination node is interconnected with each other through four bridging HMal⁻ ligands (Fig. 2). The binuclear coordination nodes are additionally connected *via* intralayer O—H$_{\text{water}}$⋯Cl and O—H$_{\text{water}}$⋯O hydrogen bonds (Table 1 and Fig. 3). Adjacent layers are linked along [001] *via* interlayer O—H⋯O=C hydrogen bonds involving two HMal⁻ ligands (Table 1 and Fig. 3).
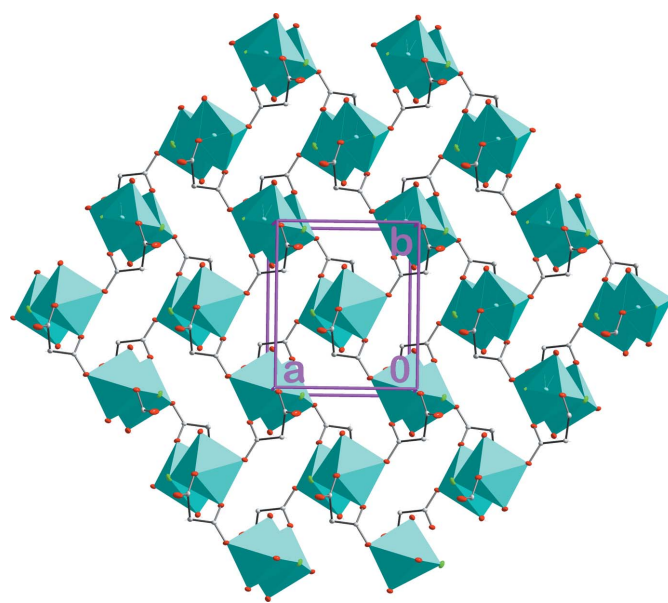

Figure 2
A view of the polymeric coordination layer in the crystal of the title compound, extending parallel to (001).

Table 2
Experimental details.

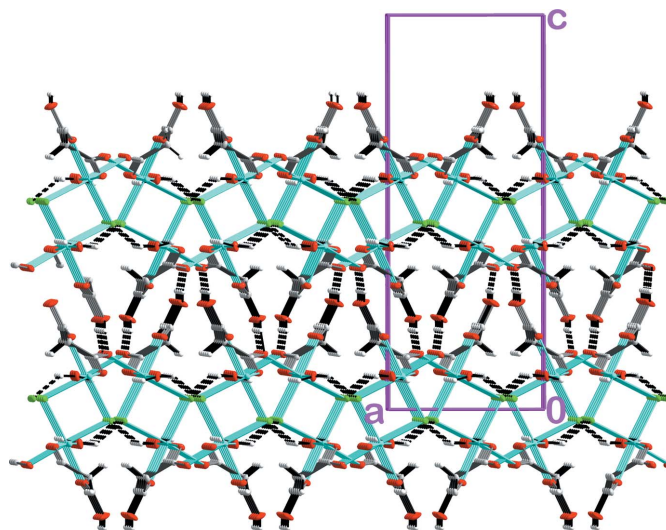| Crystal data	
Chemical formula	$[Co_2(C_3H_3O_4)_2Cl_2(H_2O)_2]$
M_r	430.90
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, b, c (Å)	7.568 (5), 8.879 (5), 19.168 (5)
V (Å^3)	1288.0 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.04
Crystal size (mm)	$0.20 \times 0.14 \times 0.07$
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.632, 0.820
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6888, 1875, 1400
R_{int}	0.055
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.116, 1.05
No. of reflections	1875
No. of parameters	91
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.05, −1.00

Computer programs: *COLLECT* (Nonius, 2000), *DENZO/SCALEPACK* (Otwinowski & Minor, 1997), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2010).

Figure 3
A view along [010] of the crystal packing of the title compound showing the inter- and intralayer hydrogen-bonding system (dashed lines).

4. Database survey

A search of the Cambridge Structural Database (Groom & Allen, 2014) revealed a number of coordination polymeric structures containing cobalt(II) malonate moieties in different coordination modes. While the most typical coordination mode of malonate ligands in polymeric structures appears to be a μ_3-bridging mode of the fully deprotonated acid involving all four oxygen atoms (usually two of them forming a chelating ring with one Co^{II} atom) (Delgado *et al.*, 2004; Xue *et al.*, 2003; Lightfoot & Snedden, 1999; Walter-Levy *et al.*, 1973; Zheng & Xie, 2004; Montney *et al.*, 2008; Fu *et al.*, 2006; Djeghri *et al.*, 2006), there are also cases of less-common coordination modes in polymeric structures such as a μ_2-bridging mode of the fully deprotonated ligand connecting two metal atoms (Gil de Muro *et al.*, 1999; Pérez-Yáñez *et al.*, 2009; Jin & Chen, 2007). Much less common in coordination polymers is a mono-deprotonated state of malonic acid (Adarsh *et al.*, 2010), while there are also few examples of non-polymeric coordination compounds (Walter-Levy *et al.*, 1973; Clarkson *et al.*, 2001; Wang *et al.*, 2005).

5. Synthesis and crystallization

The title compound was synthesized by heating together 0.104 g (1 mmol) malonic acid dissolved in 15 ml of propanol and 0.238 g (1 mmol) of CoCl$_2$·6H$_2$O dissolved in 5 ml of water. Violet crystals suitable for X-ray analysis were isolated after two weeks by slow evaporation of the solvent from the resulting mixture. Crystals were washed with small amounts of propanol and dried in air yielding 0.071 g (36%) of the title compound.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bound to O atoms were located from a difference-Fourier map and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.5\ U_{eq}(O)$. All C-bound H atoms were positioned geometrically and were also constrained to ride on their parent atoms, with C—H = 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$.

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supporting information

Crystal structure of poly[diaqua(*μ*-2-carboxyacetato-*κ*^{3}*O,O′:O″*)(2-carboxy-acetato-*κO*)di-*μ*-chlorido-dicobalt(II)]

Yasmina Bouaoud, Zouaoui Setifi, Andrii Buvailo, Vadim A. Potaskalov, Hocine Merazig and Georges Dénés

Computing details

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

Poly[diaqua(*μ*-2-carboxyacetato-*κ*^{3}*O,O′:O″*)(2-carboxyacetato-*κO*)di-*μ*-chlorido-cobalt(II)]

Crystal data

[Co$_2$(C$_3$H$_3$O$_4$)$_2$Cl$_2$(H$_2$O)$_2$]	$F(000) = 856$
$M_r = 430.90$	$D_x = 2.222$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *Kα* radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1003 reflections
$a = 7.568$ (5) Å	$\theta = 3.4$–27.6°
$b = 8.879$ (5) Å	$\mu = 3.04$ mm^{-1}
$c = 19.168$ (5) Å	$T = 296$ K
$V = 1288.0$ (12) Å^3	Block, violet
$Z = 4$	0.20 × 0.14 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer	$T_{min} = 0.632$, $T_{max} = 0.820$
Radiation source: fine-focus sealed tube	6888 measured reflections
Horizontally mounted graphite crystal monochromator	1875 independent reflections
	1400 reflections with $I > 2\sigma(I)$
Detector resolution: 9 pixels mm^{-1}	$R_{int} = 0.055$
φ scans and *ω* scans with *κ* offset	$\theta_{max} = 30.0°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -24 \rightarrow 26$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	
$wR(F^2) = 0.116$	
$S = 1.05$	Hydrogen site location: inferred from neighbouring sites
1875 reflections	H-atom parameters constrained
91 parameters	
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.9469P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -1.00$ e Å^{-3}

Special details

Experimental. The O—H H atoms were located from the difference Fourier map but constrained to ride it's parent atom, with $U_{iso} = 1.5$ U_{eq}(parent atom). Other H atoms were positioned geometrically and were also constrained to ride on their parent atoms, with C—H = 0.97 Å, and $U_{iso} = 1.2$ U_{eq}(parent atom).

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	0.57087 (6)	0.47694 (6)	0.58530 (2)	0.01449 (15)
Cl1	0.71412 (10)	0.46924 (11)	0.47183 (5)	0.0223 (2)
C1	0.4104 (4)	0.6347 (4)	0.70892 (19)	0.0177 (7)
C2	0.4303 (4)	0.7853 (4)	0.6731 (2)	0.0176 (7)
H2A	0.3323	0.7991	0.6411	0.021*
H2B	0.4237	0.8644	0.7079	0.021*
C3	0.6012 (4)	0.8016 (4)	0.63323 (18)	0.0133 (7)
O1	0.6877 (3)	0.9227 (3)	0.64044 (14)	0.0179 (5)
O2	0.5004 (3)	0.2544 (3)	0.58516 (16)	0.0276 (6)
H1O2	0.5966	0.1929	0.5746	0.041*
H2O2	0.3970	0.2004	0.5857	0.041*
O3	0.4575 (3)	0.5133 (3)	0.68488 (14)	0.0202 (6)
O4	0.3363 (4)	0.6465 (3)	0.77023 (15)	0.0321 (7)
H1O4	0.3361	0.5574	0.7994	0.048*
O5	0.6515 (3)	0.6967 (3)	0.59383 (13)	0.0175 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0156 (2)	0.0112 (2)	0.0167 (3)	−0.00042 (16)	−0.00079 (17)	−0.00210 (19)
Cl1	0.0181 (4)	0.0284 (5)	0.0204 (4)	0.0089 (3)	0.0002 (3)	−0.0038 (4)
C1	0.0123 (13)	0.0175 (19)	0.0233 (19)	−0.0019 (12)	0.0039 (13)	0.0013 (15)
C2	0.0146 (13)	0.0125 (17)	0.0257 (19)	0.0004 (12)	0.0054 (13)	0.0009 (15)
C3	0.0148 (13)	0.0099 (16)	0.0152 (17)	0.0007 (11)	0.0005 (11)	0.0014 (13)
O1	0.0206 (11)	0.0110 (12)	0.0220 (13)	−0.0028 (9)	0.0063 (10)	−0.0034 (11)
O2	0.0171 (11)	0.0177 (15)	0.0481 (19)	−0.0021 (10)	−0.0059 (12)	−0.0016 (13)
O3	0.0274 (13)	0.0133 (13)	0.0198 (14)	−0.0018 (10)	0.0038 (10)	−0.0005 (11)
O4	0.0514 (17)	0.0192 (15)	0.0257 (15)	0.0046 (13)	0.0211 (14)	0.0029 (12)
O5	0.0213 (11)	0.0116 (12)	0.0196 (13)	−0.0021 (9)	0.0052 (10)	−0.0047 (10)

Geometric parameters (Å, º)

Co1—O2	2.046 (3)	C2—C3	1.509 (4)
Co1—O5	2.051 (3)	C2—H2A	0.9700
Co1—O3	2.118 (3)	C2—H2B	0.9700
Co1—O1ⁱ	2.165 (3)	C3—O5	1.258 (4)
Co1—Cl1	2.4312 (12)	C3—O1	1.267 (4)
Co1—Cl1ⁱⁱ	2.4657 (16)	O1—Co1ⁱⁱⁱ	2.165 (3)
Cl1—Co1ⁱⁱ	2.4657 (16)	O2—H1O2	0.9325
C1—O3	1.225 (5)	O2—H2O2	0.9180
C1—O4	1.306 (4)	O4—H1O4	0.9698
C1—C2	1.511 (5)		
O2—Co1—O5	174.98 (11)	O4—C1—C2	112.4 (3)
O2—Co1—O3	92.46 (11)	C3—C2—C1	113.6 (3)
O5—Co1—O3	84.46 (10)	C3—C2—H2A	108.8
O2—Co1—O1ⁱ	90.35 (10)	C1—C2—H2A	108.8
O5—Co1—O1ⁱ	85.50 (10)	C3—C2—H2B	108.8
O3—Co1—O1ⁱ	86.33 (10)	C1—C2—H2B	108.8
O2—Co1—Cl1	95.04 (9)	H2A—C2—H2B	107.7
O5—Co1—Cl1	88.02 (7)	O5—C3—O1	122.5 (3)
O3—Co1—Cl1	172.49 (8)	O5—C3—C2	119.5 (3)
O1ⁱ—Co1—Cl1	93.10 (8)	O1—C3—C2	118.0 (3)
O2—Co1—Cl1ⁱⁱ	87.62 (8)	C3—O1—Co1ⁱⁱⁱ	124.9 (2)
O5—Co1—Cl1ⁱⁱ	96.38 (8)	Co1—O2—H1O2	111.3
O3—Co1—Cl1ⁱⁱ	90.93 (8)	Co1—O2—H2O2	136.6
O1ⁱ—Co1—Cl1ⁱⁱ	176.52 (8)	H1O2—O2—H2O2	111.2
Cl1—Co1—Cl1ⁱⁱ	89.89 (4)	C1—O3—Co1	126.2 (3)
Co1—Cl1—Co1ⁱⁱ	90.11 (4)	C1—O4—H1O4	117.0
O3—C1—O4	122.3 (4)	C3—O5—Co1	131.5 (2)
O3—C1—C2	125.3 (3)		
O2—Co1—Cl1—Co1ⁱⁱ	87.60 (8)	C2—C1—O3—Co1	−2.5 (5)
O5—Co1—Cl1—Co1ⁱⁱ	−96.39 (8)	O2—Co1—O3—C1	−158.3 (3)
O1ⁱ—Co1—Cl1—Co1ⁱⁱ	178.22 (8)	O5—Co1—O3—C1	25.7 (3)
Cl1ⁱⁱ—Co1—Cl1—Co1ⁱⁱ	0.0	O1ⁱ—Co1—O3—C1	111.5 (3)
O3—C1—C2—C3	−38.3 (5)	Cl1ⁱⁱ—Co1—O3—C1	−70.6 (3)
O4—C1—C2—C3	141.5 (3)	O1—C3—O5—Co1	166.5 (2)
C1—C2—C3—O5	46.5 (5)	C2—C3—O5—Co1	−14.4 (5)
C1—C2—C3—O1	−134.3 (4)	O3—Co1—O5—C3	−17.1 (3)
O5—C3—O1—Co1ⁱⁱⁱ	2.2 (5)	O1ⁱ—Co1—O5—C3	−103.9 (3)
C2—C3—O1—Co1ⁱⁱⁱ	−176.9 (2)	Cl1—Co1—O5—C3	162.9 (3)
O4—C1—O3—Co1	177.8 (2)	Cl1ⁱⁱ—Co1—O5—C3	73.2 (3)

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

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O2—H1*O2*⋯O5[i]	0.93	1.94	2.689 (4)	136
O2—H2*O2*⋯Cl1[iv]	0.92	2.32	3.135 (3)	147
O4—H1*O4*⋯O1[v]	0.97	1.67	2.629 (4)	169

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