

# Poly[di- $\mu$ -aqua-diaqua-di- $\mu_6$ -malonato-cobalt(II)dipotassium(I)]

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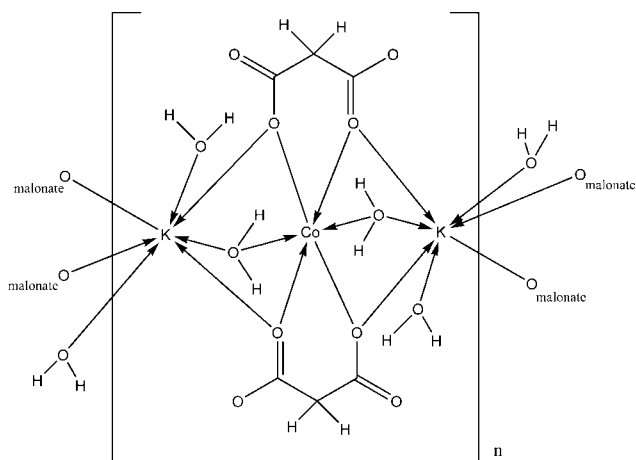
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.057; data-to-parameter ratio = 13.3.

In the title complex,  $[\text{CoK}_2(\text{C}_3\text{H}_2\text{O}_4)_2(\text{H}_2\text{O})_4]_n$ , the Co atom is located on a position with site symmetry  $2/m$ , the K atom and one water molecule are located on a mirror plane, and the malonate and one water molecule are located on a twofold rotation axis. The  $\text{K}^{\text{I}}$  atom is seven-coordinated by four carboxylate O atoms from four malonate ligands and by three water O atoms, forming a distorted polyhedron. The  $\text{Co}^{\text{II}}$  atom is in an almost octahedral environment formed by four carboxylate O atoms from two malonate ligands and two water O atoms. The structure consists of layers parallel to  $(20\bar{1})$  built up from edge-sharing  $\text{KO}_7$  and  $\text{CoO}_6$  polyhedra, which are connected by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonding including water molecules into a three-dimensional network.

## Related literature

For related structures, see: Baggio *et al.* (2003); Li *et al.* (2004); Zhao *et al.* (2007); Wang (2006).



## Experimental

### Crystal data

$[\text{CoK}_2(\text{C}_3\text{H}_2\text{O}_4)_2(\text{H}_2\text{O})_4]$   
 $M_r = 413.28$   
 Monoclinic,  $C2/m$   
 $a = 9.462$  (2) Å  
 $b = 11.014$  (3) Å  
 $c = 7.740$  (2) Å  
 $\beta = 115.65$  (2)°

$V = 727.1$  (3) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.81$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.15 \times 0.13 \times 0.10$  mm

### Data collection

Enraf–Nonius CAD-4 diffractometer  
 1825 measured reflections  
 835 independent reflections  
 813 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$   
 Standard reflections: 2; every 120 minutes  
 intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.057$   
 $S = 1.15$   
 835 reflections  
 63 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Co1–O2	2.0584 (11)	Co1–O1	2.1347 (18)
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**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–HW1 $\cdots$ O3 <sup>iv</sup>	0.81 (2)	1.91 (2)	2.7077 (17)	167 (2)
O4–HW2 $\cdots$ O3 <sup>i</sup>	0.80 (3)	2.03 (3)	2.8372 (18)	176 (3)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); 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, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5510).

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## supporting information

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**Poly[di- $\mu$ -aqua-diaqua-di- $\mu_6$ -malonato-cobalt(II)dipotassium(I)]**

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**S1. Comment**

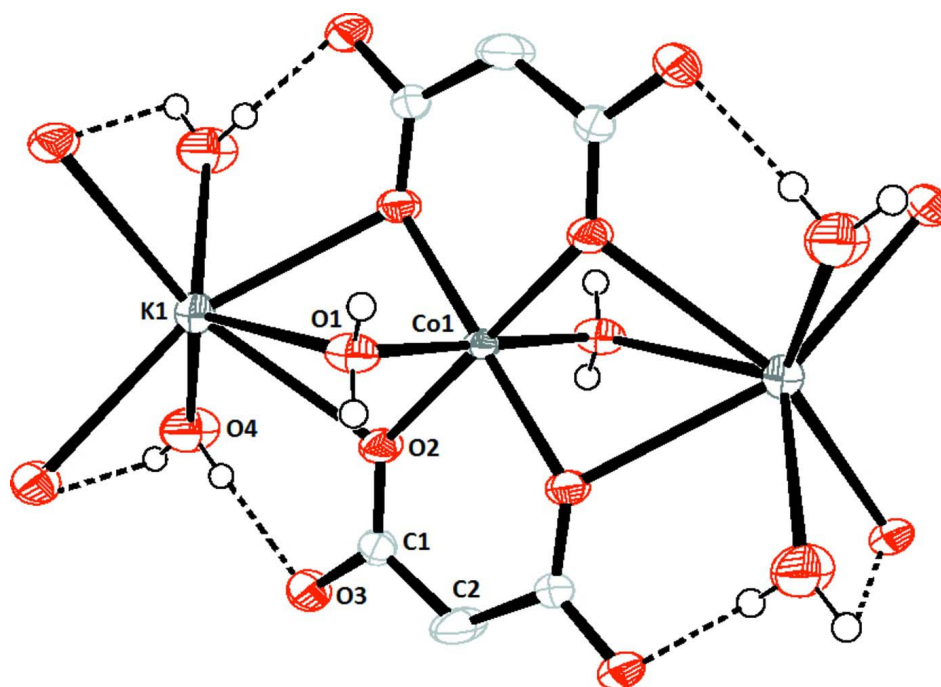
The structure of the title compound is represented in Fig. 1. The Co<sup>II</sup> cations are in a near perfect octahedral geometry with all *trans*-octahedral angles being 180° and the K ions are all in seven coordinated environment. In the quasi-regular octahedral environment of the six-coordinated Co<sup>II</sup> cation, basal coordination positions are occupied by four oxygen atoms from two malonate ligands with Co—O distances of 2.0584 (11) Å and the O—Co—O angles in the range [86.32 (5)–93.68 (5) °]. These values agree with those found in literature (Baggio *et al.*, 2003; Li *et al.*). The apical coordination position are occupied by oxygen atoms from water molecules with bond length [Co—O 2.1347 (18) Å] and an angle value of 180.00 (11) which agree with the values observed for [Co(malonate)(H<sub>2</sub>O)]<sup>2-</sup> cobalt complex (Zhao *et al.*, 2007). The potassium cation has an O7 donor set made up by four  $\mu_2$ -bridging malonate oxygen atoms and one  $\mu_2$ -bridging water oxygen atoms and two water coordinated molecules. The K cations share four oxygen atoms bridges from malonate groups and two oxygen atoms from water molecule with Co cations. There are hydrogen bonds between water molecules and carbonyl groups of the malonate anions. The cations Co<sup>II</sup> and K<sup>I</sup> are arranged in the following sequence: Co—K—K—Co. The metal atoms are found at linear positions [K—Co—K, 180.00 (0)°] as shown in Fig. 2. The Co—K distance is 3.5726 (13) Å. Two K atoms are found to be very close together, having a distance of 4.2086 (14) Å, which is a short metal–metal distance for these types of complexes. The insertion of two polyhedra of KO<sub>7</sub> between two polyhedra of CoO<sub>6</sub> results in long Co—Co distances. These two types of geometries form zigzag layers parallel to the *ac*-plane and alternating with malonate groups along the *b* axis. The water oxygen atoms provide bridges between K cations. The different polyhedra are still bound to each other through edge-sharing with a compact layer structure defining narrow crossed channels.

**S2. Experimental**

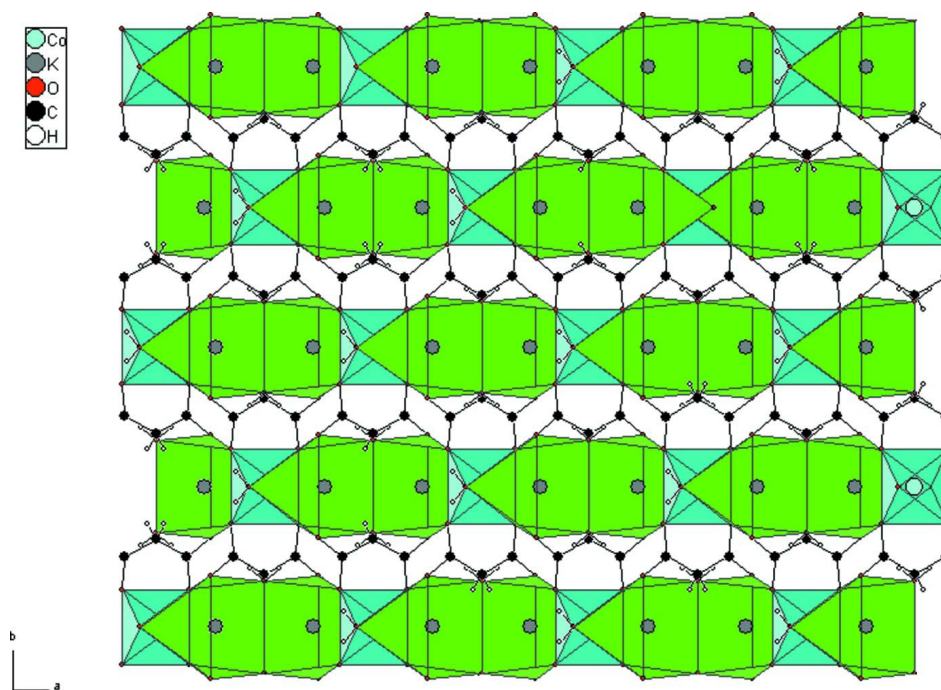
In a round bottomed flask, cobalt acetate tetrahydrate (0.4982 g, 2 mmol) dissolved in a mixture of water and methanol (10 ml, 1:1) was introduced. Imidazole (0.2720 g, 4 mmol) dissolved in 10 ml of the same mixture was added. The solution turn pink. After 10 mn of stirring, 10 ml of a mixture of methanol and water (10 ml, 1:1) containing malonic acid (0.2081 g, 2 mmol) and KOH (0.2240 g, 4 mmol) was added to the pink solution. After 2 h under stirring, the suspension was filtered off and the precipitate was washed with water and diethyl ether before drying under P<sub>2</sub>O<sub>5</sub>. The compound was recrystallized in a mixture of water and dimethylformamide (1/1). After one week, suitable pink crystals for X-ray analyses was obtained. Yield: 72%. m.p. 228±1°C. Anal. Calc. For [C<sub>6</sub>H<sub>12</sub>O<sub>12</sub>K<sub>2</sub>Co]<sub>n</sub> (%): C, 17.44; H, 2.93. Found: C, 17.44; H, 2.93. Selected IR data (cm<sup>-1</sup>, KBr pellet): 3216, 1637, 1600, 1582, 1197, 764.

**S3. Refinement**

The H atoms of the water molecules were located in a Fourier difference map and freely refined. H atoms of the CH<sub>2</sub> groups were geometrically placed and refined with a riding model with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

**Figure 1**

An *ORTEP* view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level. Broken lines indicate hydrogen bonds.

**Figure 2**

Projection of the structure onto the *c* axis showing the polyhedra layers connected by the organics molecules.

Poly[di- $\mu$ -aqua-diaqua-di- $\mu_6$ -malonato-cobalt(II)dipotassium]

## Crystal data

[CoK<sub>2</sub>(C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>] $M_r = 413.28$ Monoclinic,  $C2/m$ Hall symbol:  $-C\ 2y$  $a = 9.462\ (2)\ \text{\AA}$  $b = 11.014\ (3)\ \text{\AA}$  $c = 7.740\ (2)\ \text{\AA}$  $\beta = 115.65\ (2)^\circ$  $V = 727.1\ (3)\ \text{\AA}^3$  $Z = 2$  $F(000) = 418$  $D_x = 1.888\ \text{Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$ 

Cell parameters from 25 reflections

 $\theta = 11\text{--}15^\circ$  $\mu = 1.81\ \text{mm}^{-1}$  $T = 293\ \text{K}$ 

Prism, pink

 $0.15 \times 0.13 \times 0.10\ \text{mm}$ 

## Data collection

Enraf–Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scans

1825 measured reflections

835 independent reflections

813 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.022$  $\theta_{\text{max}} = 27.0^\circ$ ,  $\theta_{\text{min}} = 2.9^\circ$  $h = -12 \rightarrow 12$  $k = -1 \rightarrow 14$  $l = -9 \rightarrow 9$ 

2 standard reflections every 120 min

intensity decay: none

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.022$  $wR(F^2) = 0.057$  $S = 1.15$ 

835 reflections

63 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from

neighbouring sites

H atoms treated by a mixture of independent

and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 0.6549P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.33\ \text{e \AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.30\ \text{e \AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.045 (2)

## 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.0000	0.0000	0.0000	0.01988 (16)	
K1	-0.27538 (6)	0.0000	-0.49356 (7)	0.03100 (18)	
O1	0.0747 (2)	0.0000	-0.2237 (3)	0.0308 (4)	

O2	0.15473 (12)	0.13440 (10)	0.15312 (16)	0.0290 (3)	
O3	0.24932 (14)	0.31676 (10)	0.26017 (17)	0.0334 (3)	
O4	-0.5000	-0.16509 (19)	-0.5000	0.0479 (5)	
C1	0.14331 (17)	0.24844 (13)	0.1464 (2)	0.0234 (3)	
C2	0.0000	0.3130 (2)	0.0000	0.0519 (8)	
H1	-0.0371	0.3657	0.0720	0.062*	0.50
H2	0.0371	0.3657	-0.0720	0.062*	0.50
HW1	0.134 (2)	0.055 (2)	-0.217 (3)	0.054 (7)*	
HW2	-0.431 (3)	-0.211 (2)	-0.435 (4)	0.066 (8)*	

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0200 (2)	0.0129 (2)	0.0208 (2)	0.000	0.00322 (16)	0.000
K1	0.0360 (3)	0.0267 (3)	0.0248 (3)	0.000	0.0079 (2)	0.000
O1	0.0357 (9)	0.0200 (7)	0.0416 (10)	0.000	0.0215 (8)	0.000
O2	0.0261 (5)	0.0169 (5)	0.0309 (6)	-0.0021 (4)	0.0001 (4)	0.0004 (4)
O3	0.0328 (6)	0.0228 (6)	0.0330 (6)	-0.0090 (4)	0.0034 (5)	-0.0032 (5)
O4	0.0287 (9)	0.0348 (10)	0.0599 (13)	0.000	0.0000 (9)	0.000
C1	0.0253 (7)	0.0185 (7)	0.0233 (7)	-0.0039 (6)	0.0076 (6)	-0.0002 (5)
C2	0.0451 (15)	0.0169 (11)	0.0555 (17)	0.000	-0.0141 (13)	0.000

*Geometric parameters (Å, °)*

Co1—O2 <sup>i</sup>	2.0584 (11)	K1—O1 <sup>vii</sup>	3.4628 (19)
Co1—O2	2.0584 (11)	K1—K1 <sup>iv</sup>	4.2086 (14)
Co1—O2 <sup>ii</sup>	2.0584 (11)	K1—HW2	2.89 (3)
Co1—O2 <sup>iii</sup>	2.0584 (11)	O1—K1 <sup>vii</sup>	3.4628 (19)
Co1—O1	2.1347 (18)	O1—HW1	0.81 (2)
Co1—O1 <sup>i</sup>	2.1347 (18)	O2—C1	1.2598 (18)
Co1—K1 <sup>i</sup>	3.5726 (13)	O2—K1 <sup>i</sup>	2.7987 (13)
Co1—K1	3.5726 (13)	O3—C1	1.2582 (18)
K1—O4	2.7811 (15)	O3—K1 <sup>viii</sup>	2.8541 (14)
K1—O4 <sup>iv</sup>	2.7811 (15)	O4—K1 <sup>iv</sup>	2.7810 (15)
K1—O2 <sup>iii</sup>	2.7987 (13)	O4—HW2	0.80 (3)
K1—O2 <sup>i</sup>	2.7987 (13)	C1—C2	1.5157 (19)
K1—O3 <sup>v</sup>	2.8541 (14)	C2—C1 <sup>iii</sup>	1.5157 (19)
K1—O3 <sup>vi</sup>	2.8541 (14)	C2—H1	0.9700
K1—O1	3.057 (2)	C2—H2	0.9700
O2 <sup>i</sup> —Co1—O2	180.00 (11)	O3 <sup>v</sup> —K1—O1 <sup>vii</sup>	49.62 (3)
O2 <sup>i</sup> —Co1—O2 <sup>ii</sup>	88.03 (6)	O3 <sup>vi</sup> —K1—O1 <sup>vii</sup>	49.62 (3)
O2—Co1—O2 <sup>ii</sup>	91.97 (6)	O1—K1—O1 <sup>vii</sup>	72.74 (6)
O2 <sup>i</sup> —Co1—O2 <sup>iii</sup>	91.97 (6)	O4—K1—Co1	102.54 (2)
O2—Co1—O2 <sup>iii</sup>	88.03 (6)	O4 <sup>iv</sup> —K1—Co1	102.54 (2)
O2 <sup>ii</sup> —Co1—O2 <sup>iii</sup>	180.0	O2 <sup>iii</sup> —K1—Co1	35.11 (2)
O2 <sup>i</sup> —Co1—O1	86.32 (5)	O2 <sup>i</sup> —K1—Co1	35.11 (2)
O2—Co1—O1	93.68 (5)	O3 <sup>v</sup> —K1—Co1	118.77 (3)

O2 <sup>ii</sup> —Co1—O1	93.68 (5)	O3 <sup>vi</sup> —K1—Co1	118.77 (3)
O2 <sup>iii</sup> —Co1—O1	86.32 (5)	O1—K1—Co1	36.53 (4)
O2 <sup>i</sup> —Co1—O1 <sup>i</sup>	93.68 (5)	O1 <sup>vii</sup> —K1—Co1	109.27 (4)
O2—Co1—O1 <sup>i</sup>	86.32 (5)	O4—K1—K1 <sup>iv</sup>	40.83 (3)
O2 <sup>ii</sup> —Co1—O1 <sup>i</sup>	86.32 (5)	O4 <sup>iv</sup> —K1—K1 <sup>iv</sup>	40.83 (3)
O2 <sup>iii</sup> —Co1—O1 <sup>i</sup>	93.68 (5)	O2 <sup>iii</sup> —K1—K1 <sup>iv</sup>	91.05 (3)
O1—Co1—O1 <sup>i</sup>	180.00 (8)	O2 <sup>i</sup> —K1—K1 <sup>iv</sup>	91.05 (3)
O2 <sup>i</sup> —Co1—K1 <sup>i</sup>	128.56 (3)	O3 <sup>v</sup> —K1—K1 <sup>iv</sup>	110.98 (3)
O2—Co1—K1 <sup>i</sup>	51.44 (3)	O3 <sup>vi</sup> —K1—K1 <sup>iv</sup>	110.98 (3)
O2 <sup>ii</sup> —Co1—K1 <sup>i</sup>	51.44 (3)	O1—K1—K1 <sup>iv</sup>	143.21 (4)
O2 <sup>iii</sup> —Co1—K1 <sup>i</sup>	128.56 (3)	O1 <sup>vii</sup> —K1—K1 <sup>iv</sup>	144.05 (4)
O1—Co1—K1 <sup>i</sup>	121.53 (5)	Co1—K1—K1 <sup>iv</sup>	106.68 (3)
O1 <sup>i</sup> —Co1—K1 <sup>i</sup>	58.47 (5)	O4—K1—HW2	16.2 (5)
O2 <sup>i</sup> —Co1—K1	51.44 (3)	O4 <sup>iv</sup> —K1—HW2	95.2 (5)
O2—Co1—K1	128.56 (3)	O2 <sup>iii</sup> —K1—HW2	107.8 (5)
O2 <sup>ii</sup> —Co1—K1	128.56 (3)	O2 <sup>i</sup> —K1—HW2	57.0 (5)
O2 <sup>iii</sup> —Co1—K1	51.44 (3)	O3 <sup>v</sup> —K1—HW2	74.4 (6)
O1—Co1—K1	58.47 (5)	O3 <sup>vi</sup> —K1—HW2	150.2 (5)
O1 <sup>i</sup> —Co1—K1	121.53 (5)	O1—K1—HW2	111.6 (5)
K1 <sup>i</sup> —Co1—K1	180.0	O1 <sup>vii</sup> —K1—HW2	123.8 (6)
O4—K1—O4 <sup>iv</sup>	81.66 (7)	Co1—K1—HW2	91.0 (5)
O4—K1—O2 <sup>iii</sup>	111.08 (4)	K1 <sup>iv</sup> —K1—HW2	54.9 (5)
O4 <sup>iv</sup> —K1—O2 <sup>iii</sup>	70.62 (3)	Co1—O1—K1	85.00 (6)
O4—K1—O2 <sup>i</sup>	70.62 (3)	Co1—O1—K1 <sup>vii</sup>	167.75 (8)
O4 <sup>iv</sup> —K1—O2 <sup>i</sup>	111.08 (4)	K1—O1—K1 <sup>vii</sup>	107.26 (6)
O2 <sup>iii</sup> —K1—O2 <sup>i</sup>	63.86 (5)	Co1—O1—HW1	114.1 (18)
O4—K1—O3 <sup>v</sup>	78.97 (4)	K1—O1—HW1	124.1 (16)
O4 <sup>iv</sup> —K1—O3 <sup>v</sup>	137.16 (4)	K1 <sup>vii</sup> —O1—HW1	59.3 (17)
O2 <sup>iii</sup> —K1—O3 <sup>v</sup>	152.22 (4)	C1—O2—Co1	131.78 (10)
O2 <sup>i</sup> —K1—O3 <sup>v</sup>	97.86 (4)	C1—O2—K1 <sup>i</sup>	123.99 (10)
O4—K1—O3 <sup>vi</sup>	137.16 (4)	Co1—O2—K1 <sup>i</sup>	93.45 (4)
O4 <sup>iv</sup> —K1—O3 <sup>vi</sup>	78.97 (4)	C1—O3—K1 <sup>viii</sup>	128.27 (10)
O2 <sup>iii</sup> —K1—O3 <sup>vi</sup>	97.86 (4)	K1—O4—K1 <sup>iv</sup>	98.34 (7)
O2 <sup>i</sup> —K1—O3 <sup>vi</sup>	152.22 (4)	K1—O4—HW2	89.5 (19)
O3 <sup>v</sup> —K1—O3 <sup>vi</sup>	90.00 (5)	K1 <sup>iv</sup> —O4—HW2	146 (2)
O4—K1—O1	127.30 (3)	O3—C1—O2	122.62 (14)
O4 <sup>iv</sup> —K1—O1	127.30 (3)	O3—C1—C2	115.27 (15)
O2 <sup>iii</sup> —K1—O1	58.47 (4)	O2—C1—C2	122.11 (15)
O2 <sup>i</sup> —K1—O1	58.47 (4)	C1 <sup>iii</sup> —C2—C1	124.1 (2)
O3 <sup>v</sup> —K1—O1	94.50 (4)	C1 <sup>iii</sup> —C2—H1	106.3
O3 <sup>vi</sup> —K1—O1	94.50 (4)	C1—C2—H1	106.3
O4—K1—O1 <sup>vii</sup>	127.77 (3)	C1 <sup>iii</sup> —C2—H2	106.3
O4 <sup>iv</sup> —K1—O1 <sup>vii</sup>	127.77 (3)	C1—C2—H2	106.3
O2 <sup>iii</sup> —K1—O1 <sup>vii</sup>	118.90 (4)	H1—C2—H2	106.4
O2 <sup>i</sup> —K1—O1 <sup>vii</sup>	118.90 (4)		

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

*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>
O1—HW1 $\cdots$ O3 <sup>ix</sup>	0.81 (2)	1.91 (2)	2.7077 (17)	167 (2)
O4—HW2 $\cdots$ O3 <sup>i</sup>	0.80 (3)	2.03 (3)	2.8372 (18)	176 (3)

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