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# *catena*-Poly[[[diaquacobalt(II)]-$\mu$-tartrato-$\kappa^4O,O':O'',O'''$] monohydrate]

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**Key indicators**

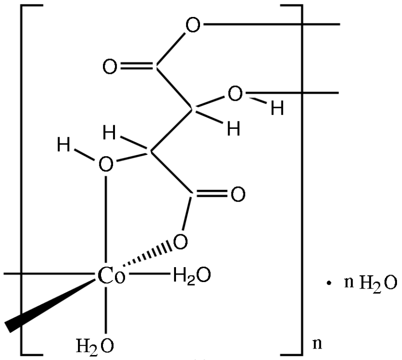
Single-crystal X-ray study
$T$ = 295 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.030
$wR$ factor = 0.074
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title Co$^{II}$ polymeric complex bridged by tartrate dianions, $\{[Co(C_4H_4O_6)(H_2O)_2]\cdot H_2O\}_n$, the Co$^{II}$ atom is coordinated by two tartrate dianions and two water molecules to give a distorted octahedral geometry. The hydroxyl O atom and one O atom of each carboxyl group chelate to the Co$^{II}$ atom, but the other O atom of this carboxyl group is uncoordinated. The polymeric chains are linked to each other *via* hydrogen bonds to form cavities which are filled with solvent water molecules.

## Comment

The crystal structures of transition metal complexes with dicarboxylate ligands show versatile coordination modes of the carboxylate group. In the title cobalt(II) complex, (I), the hydroxyl and carboxyl groups of the tartrate dianion form a chelate coordination to the Co$^{II}$ atom, but the other carboxyl O atom is free uncoordinated. A search of the Cambridge Structural Database (Version 5.25; Allen, 2002) indicates that this is an unusual coordination mode for the tartrate anion.



(I)

The complex is polymeric; the structure of a fragment of (I) is illustrated in Fig. 1. The six-coordinated Co$^{II}$ atom is surrounded by two tartrate dianions and two water molecules in a distorted octahedral geometry. Two water molecules coordinate to the Co$^{II}$ atom in a *cis* configuration with a normal O7—Co—O8 bond angle [87.48 (7)]. Two tartrate dianions chelate to the Co$^{II}$ atom with an unusual coordination mode; the hydroxyl O atom and one O atom of the carboxyl group are involved in the chelate bonding but the other O atom of the carboxyl group is uncoordinated. Thus, the carboxyl group binds in a monodentate manner to the Co atom in an *anti* configuration. Both chelate rings about the Co atom have similar envelope conformations, the Co atom being in the flap position and out of the mean planes formed by the other four atoms by 0.352 (3) (O3-containing ring) and 0.486 (3) Å (O4$^{i}$-containing ring) [symmetry code: (i) $-x+\frac{1}{2}$,

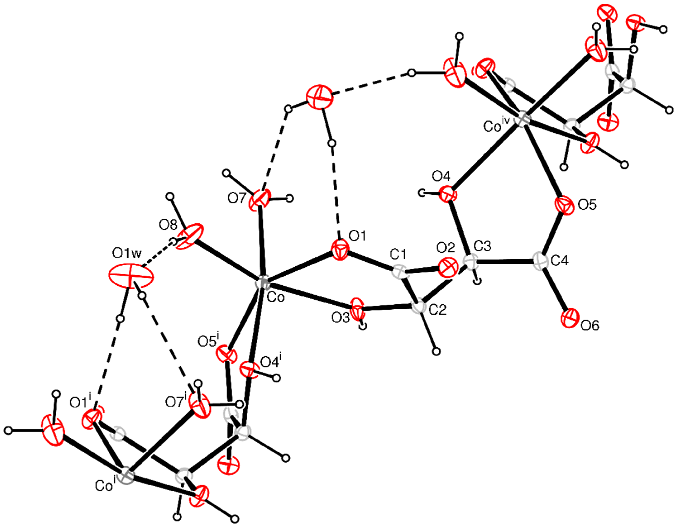


**Figure 1**
The structure of a fragment of (I) shown with 40% probability displacement ellipsoids. Dashed lines indicate the hydrogen bonding. [Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, z$].

$y+\frac{1}{2}, z$]. The O1—Co—O5$^{i}$ angle of 149.73 (6)° shows the degree of distortion of the octahedral coordination geometry. The tartrate dianion displays a *gauche* conformation with the C1—C2—C3—C4 torsion angle of 67.0 (2)°. Each tartrate bridges two Co$^{II}$ atoms to form one-dimensional polymeric chains (Fig. 1) extending along the *b* axis.

The uncoordinated carboxyl O atoms (O2 and O6) are hydrogen bonded with the hydroxyl groups and coordinated water molecules of neighboring polymeric chains (Table 2). The coordinated water (O7) is also hydrogen bonded to the carboxyl group of the neighboring polymeric chain, with an O7—H7*B*—O1$^{iii}$ angle of 180° [symmetry code: (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, 1-z$]. These interchain hydrogen bonds lead to a cavity structure in (I), as shown in Fig. 2. The uncoordinated water molecules hydrogen bond with coordinated water molecules and carboxyl groups and occupy the cavities (Table 2).

## Experimental

An ethanol/water solution (6 ml, 1:1) of $Co(CH_3COO)_2\cdot 4H_2O$ (0.18 g, 1 mmol) was mixed with an aqueous solution (4 ml) containing dibromosuccinic acid (0.55 g, 2 mmol) and NaOH (0.16 g, 4 mmol). The mixture was refluxed for 5 h and filtered. Red single crystals of (I) were obtained from the filtrate after 3 d. Analysis found: C 18.35, H 4.20%; calculated for (I): C 18.40, H 3.86%. This suggested that dibromosuccinic acid hydrolysed during the refluxing of the solution.

### *Crystal data*

$[Co(C_4H_4O_6)(H_2O)_2]\cdot H_2O$
$M_r = 261.05$
Orthorhombic, *Pbca*
$a = 10.0472$ (4) Å
$b = 11.3090$ (5) Å
$c = 14.9321$ (5) Å
$V = 1696.64$ (12) Å$^3$
$Z = 8$
$D_x = 2.044$ Mg m$^{-3}$

Mo *Kα* radiation
Cell parameters from 12622 reflections
$\theta = 3.0$–26.0°
$\mu = 2.05$ mm$^{-1}$
$T = 295$ (2) K
Prism, red
0.32 × 0.18 × 0.10 mm

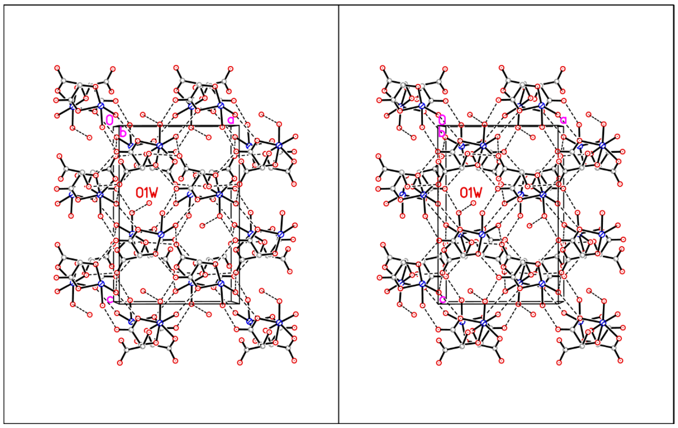


**Figure 2**
A stereoview of the unit-cell packing in (I), showing the cavity structure formed by the hydrogen-bond network (dashed lines). H atoms have been omitted for clarity.

### *Data collection*

Rigaku R-AXIS RAPID diffractometer
*ω* scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.514$, $T_{max} = 0.812$
14995 measured reflections

1947 independent reflections
1766 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -19 \rightarrow 19$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.074$
$S = 1.14$
1947 reflections
127 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 1.8309P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å$^{-3}$
$\Delta\rho_{min} = -0.52$ e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co—O1 | 2.1176 (16) | Co—O5$^{i}$ | 2.0628 (16) |
| Co—O3 | 2.1171 (15) | Co—O7 | 2.1093 (17) |
| Co—O4$^{i}$ | 2.1195 (15) | Co—O8 | 2.0007 (19) |

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

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O7$^{i}$ | 0.81 | 2.46 | 3.123 (3) | 139 |
| O1*W*—H1*B*···O1$^{i}$ | 0.95 | 2.12 | 3.059 (3) | 170 |
| O3—H3*A*···O2$^{ii}$ | 0.82 | 1.86 | 2.678 (2) | 176 |
| O4—H4*A*···O6$^{ii}$ | 0.87 | 1.74 | 2.606 (2) | 173 |
| O7—H7*A*···O6$^{ii}$ | 0.83 | 1.90 | 2.728 (2) | 171 |
| O7—H7*B*···O1$^{iii}$ | 0.86 | 2.00 | 2.863 (2) | 180 |
| O8—H8*A*···O1*W* | 0.85 | 1.86 | 2.686 (3) | 165 |
| O8—H8*B*···O2$^{iii}$ | 0.87 | 1.82 | 2.670 (3) | 166 |

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

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.98 Å, and were included in the final cycles of refinement in the riding model, with $U_{iso}(H) = 1.2U_{eq}$ of the carrier atoms. H atoms on O atoms were located in a difference Fourier map and were refined as riding in their as-found positions relative to O atoms, with fixed isotropic displacement parameters of 0.06 Å$^2$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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