



Crystal structure of *catena*-poly[[[diaquabis(2,4,6-trimethylbenzoato- κ O)cobalt(II)]- μ -aqua- κ^2 O:O] dihydrate]

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Crystal structure of *catena*-poly[[[diaquabis(2,4,6-trimethylbenzoato- κ O)cobalt(II)]- μ -aqua- κ^2 O:O] dihydrate]

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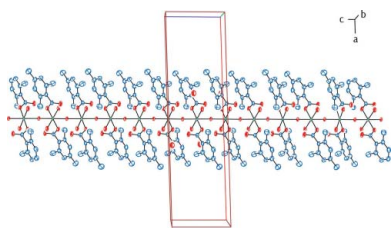
The asymmetric unit of the title one-dimensional polymeric compound, $\{[\text{Co}(\text{C}_{10}\text{H}_{11}\text{O}_2)_2(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}\}_n$, contains one Co^{II} cation situated on a centre of inversion, one-half of a coordinating water molecule, one 2,4,6-trimethylbenzoate (TMB) anion together with one coordinating and one non-coordinating water molecule; the TMB anion acts as a monodentate ligand. In the anion, the carboxylate group is twisted away from the attached benzene ring by $84.9(2)^\circ$. The Co^{II} atom is coordinated by two TMB anions and two water molecules in the basal plane, while another water molecule bridges the Co^{II} atoms in the axial directions, forming polymeric chains running along [001]. The coordination environment for the Co^{II} cation is a slightly distorted octahedron. The coordinating and bridging water molecules link to the carboxylate groups *via* intra- and intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, enclosing $S(6)$ ring motifs, while the coordinating, bridging and non-coordinating water molecules link to the carboxylate groups and the coordinating water molecules link to the non-coordinating water molecules *via* $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, enclosing $R_2^2(8)$ and $R_3^3(8)$ ring motifs. Weak $\text{C}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \pi$ interactions may further stabilize the crystal structure.

1. Chemical context

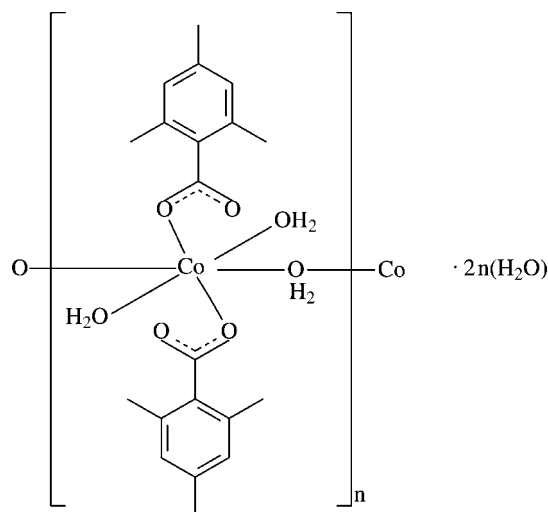
Transition metal complexes with ligands of biochemical interest, such as imidazole and some N-protected amino acids, show interesting physical and/or chemical properties, through which they may find applications in biological systems (Antolini *et al.*, 1982). Some benzoic acid derivatives, such as 4-aminobenzoic acid, have been extensively reported in coordination chemistry, as bifunctional organic ligands, due to the varieties of their coordination modes (Chen & Chen, 2002; Amiraslanov *et al.*, 1979; Hauptmann *et al.*, 2000).

The structure–function–coordination relationships of the arylcarboxylate ion in Zn^{II} complexes of benzoic acid derivatives change depending on the nature and position of the substituted groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the pH and temperature of the synthesis (Shnulin *et al.*, 1981; Nadzhafov *et al.*, 1981; Antsyshkina *et al.*, 1980; Adiwidjaja *et al.*, 1978). When pyridine and its derivatives are used instead of water molecules, the structure is completely different (Catterick *et al.*, 1974).

The solid-state structures of anhydrous zinc(II) carboxylates include one-dimensional (Guseinov *et al.*, 1984; Clegg *et al.*, 1986*a*), two-dimensional (Clegg *et al.*, 1986*b*, 1987) and



three-dimensional (Capilla & Aranda, 1979) polymeric motifs of different types, while discrete monomeric complexes with octahedral or tetrahedral coordination geometry are found if water or other donor molecules coordinate to the Zn^{II} cation (van Niekerk *et al.*, 1953; Usabaliev *et al.*, 1992).



The structures of some mononuclear polymeric complexes obtained from the reactions of transition metal(II) ions with nicotinamide (NA) and/or some benzoic acid derivatives as ligands have been determined, *e.g.* $\{Mn(C_{11}H_{14}NO_2)_2(H_2O)_3 \cdot 2H_2O\}_n$ [(II); Hökelek *et al.*, 2009], $[Mn(C_7H_4FO_2)_2(H_2O)]_n$ [(III); Necefoğlu *et al.*, 2011], $\{[Pb(C_9H_9O_2)_2(C_6H_6N_2O)] \cdot H_2O\}_n$ [(IV); Hökelek *et al.*, 2011], $\{[Pb(C_7H_5O_3)_2(C_6H_6N_2O)]H_2O\}_n$ [(V); Zaman *et al.*, 2012] and $\{[Zn(C_7H_4ClO_2)_2 \cdot (H_2O)]_n\}$ [(VI); Bozkurt *et al.*, 2013], where the transition metal(II) cations are bridged by water molecules in (II), 4-fluorobenzoate anions in (III), nicotinamide ligands in (IV), 3-hydroxybenzoate anions in (V) and 3-chlorobenzoate anions in (VI). The synthesis and structure determination of the title compound, (I), a one-dimensional polymeric cobalt(II) complex with two 2,4,6-trimethylbenzoate (TMB)

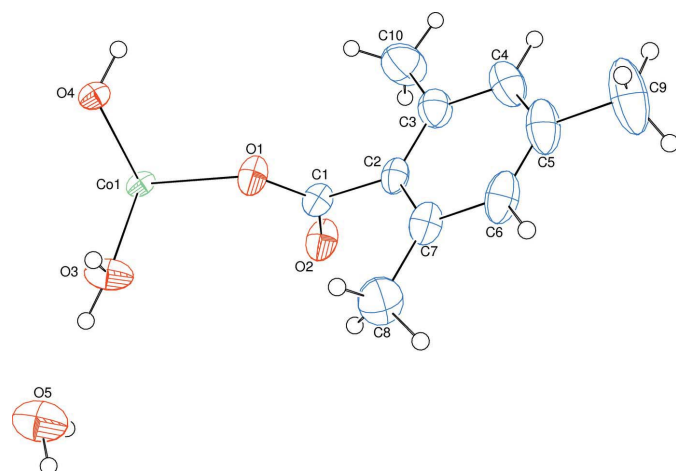


Figure 1
The asymmetric unit of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

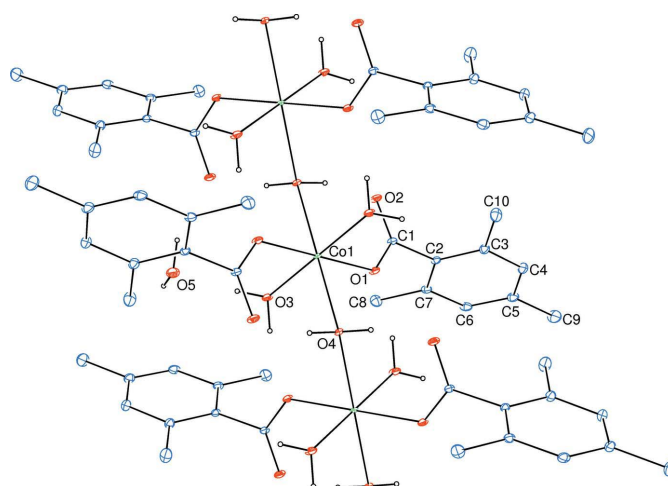


Figure 2
Partial view of the polymeric chain of the title compound. H atoms of the 2,4,6-trimethylbenzoate (TMB) anions have been omitted for clarity.

ligands and four coordinating and two non-coordinating water molecules, was undertaken in order to compare the results obtained with those reported previously. Its crystal structure is reported herein.

2. Structural commentary

The asymmetric unit of the title one-dimensional polymeric compound, (I), contains one Co^{II} cation situated on a centre of inversion, one-half of a coordinating water molecule, one 2,4,6-trimethylbenzoate (TMB) anion together with the one coordinating and one non-coordinating water molecules; the TMB anion acts as a monodentate ligand (Fig. 1).

The Co^{II} atom is coordinated by two TMB anions and two water molecules in the basal plane while another water molecule bridges the Co^{II} atoms in the axial directions, resulting in a slightly distorted octahedral coordination sphere around each Co^{2+} cation, and forming polymeric chains (Fig. 2) running along [001] (Figs. 3 and 4). The cobalt cation is formally Co^{2+} within the structure, in line with the presence of

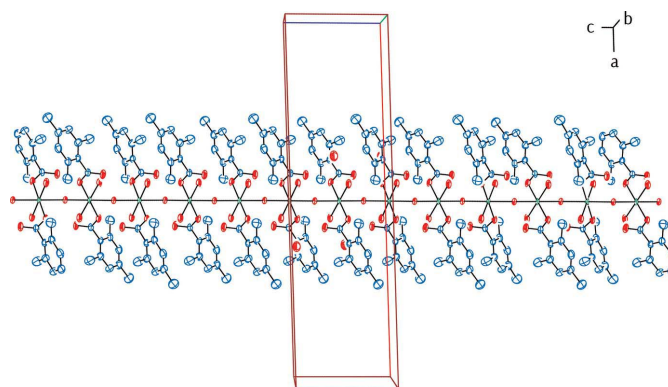


Figure 3
A partial packing diagram of the title one-dimensional polymeric compound in a view approximately along the *b* axis, where the *c* axis is horizontal and the *a* axis is vertical. H atoms have been omitted for clarity.

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

Cg1 is the centroid of the C2–C7 ring.

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O3–H31···O1 ⁱ	0.80 (2)	1.90 (2)	2.697 (3)	170 (5)
O3–H32···O5	0.82 (3)	1.91 (3)	2.724 (5)	174 (3)
O4–H41···O2 ⁱⁱ	0.83 (3)	1.82 (3)	2.622 (3)	164 (4)
O5–H52···O2 ⁱⁱⁱ	0.82 (3)	1.98 (4)	2.726 (4)	151 (6)
C10–H10C···O5 ^{iv}	0.96	2.59	3.466 (7)	152
C6–H6···Cg1 ^v	0.93	3.28	4.063 (4)	143
C9–H9A···Cg1 ^v	0.96	3.40	3.961 (7)	120

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

bridging water molecules rather than bridging hydroxide groups. This is confirmed by softness-sensitive BVS calculations (Adams, 2001), which identify the BVS for the Co atom to be 2.05 (5).

The two carboxylate O atoms (O1 and O1ⁱ) of the two symmetry-related TMB anions and the two symmetry-related water O atoms (O3 and O3ⁱ) around the Co^{II} cation form a slightly distorted square-planar arrangement with an average Co1–O bond length of 2.058 (2) Å. The slightly distorted octahedral coordination is completed by the symmetry-related bridging O atoms (O4 and O4ⁱ) with a Co1–O4 bond length of 2.2060 (11) Å in the axial directions (Fig. 2) [symmetry code: (i) $1 - x, 1 - y, 1 - z$]. The Co–O bond lengths are in the range of 2.041 (2)–2.2060 (11) Å. Among the Co–O coordinations the Co1–O3 bond [2.041 (2) Å] is the shortest and the Co1–O4 bond [2.2060 (11) Å] is the longest, probably as a result of the bidentate bridging coordination of O4

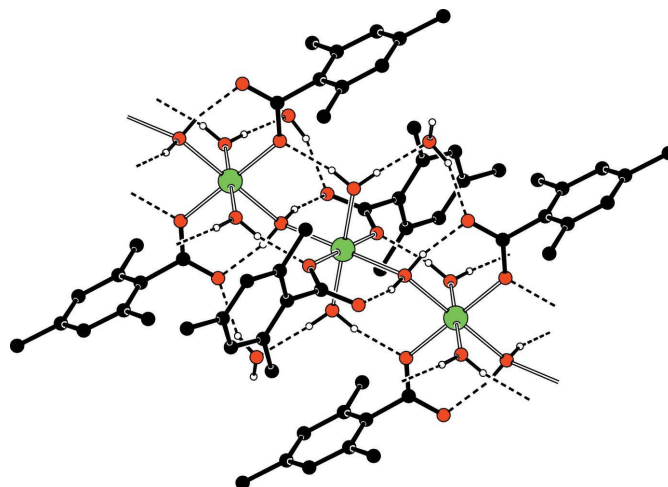


Figure 5
Part of the crystal structure. Intramolecular and intermolecular O–H···O hydrogen bonds, enclosing $S(6)$, $R_2^2(8)$ and $R_3^3(8)$ ring motifs, are shown as dashed lines. H atoms not involved in classical hydrogen bonds have been omitted for clarity.

with a very wide Co1–O4–Co1ⁱⁱ bond angle of 132.95 (13)° [symmetry code: (ii) $1 - x, y, \frac{1}{2} - z$]. The Co1 atom lies 0.2077 (1) Å above the carboxylate (O1/O2/C1) group, which makes a dihedral angle of 84.9 (2)° with the adjacent benzene (C2–C7) ring.

Neighboring Co^{II} atoms are bridged by H₂O molecules (Fig. 2) and they are also coordinated by monodentate carboxylate groups. The non-coordinating oxygen atoms of the carboxylate groups interact with the bridging water molecules *via* short hydrogen bonds (Table 1 and Fig. 5),

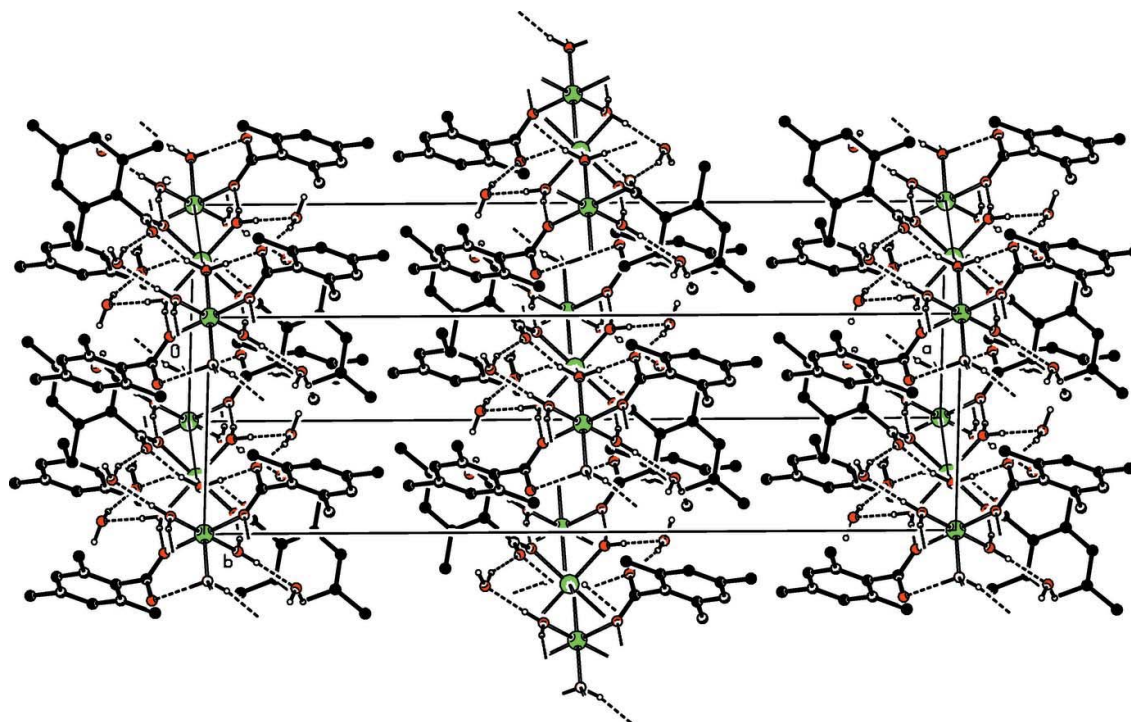


Figure 4
View of the hydrogen bonding and packing of the title one-dimensional polymeric compound along the *c* axis. H atoms not involved in classical hydrogen bonds have been omitted for clarity.

increasing the Lewis basicity of the bridging water molecules by attracting the protons of the water molecules to the oxygen atoms of the carboxylate groups. Intramolecular $O-H_{\text{brdW}} \cdots O_c$ and intermolecular $O-H_{\text{coordW}} \cdots O_c$ (brdW = bridging water, coordW = coordinating water and c = carboxylate) hydrogen bonds (Table 1) link the bridging and coordinating water molecules to the carboxylate oxygen atoms, enclosing S(6) ring motifs (Fig. 5).

3. Supramolecular features

In the crystal, $O-H_{\text{coordW}} \cdots O_c$ and $O-H_{\text{coordW}} \cdots O_{\text{noncoordW}}$, $O-H_{\text{noncoordW}} \cdots O_c$, $O-H_{\text{brdW}} \cdots O_c$ (noncoordW = non-coordinating water) hydrogen bonds (Table 1) link the molecules, enclosing $R_2^2(8)$ and $R_3^3(8)$ ring motifs, respectively (Fig. 5). $O-H \cdots O$ hydrogen bonds (Table 1) also link the hydrogen-bonded polymeric chains running along [001] into networks parallel to (011) (Fig. 4). The crystal structure is further stabilized by weak $C-H \cdots O$ and $C-H \cdots \pi$ interactions (Table 1).

4. Comparison with related structures

In the crystal structure of a similar complex, *catena*-poly[[[diaquabis[4-(diethylamino)benzoato- κO^I]manganese(II)]- μ -aqua]dihydrate], $\{[Mn(C_{10}H_{11}NO_2)_2(H_2O)_3] \cdot 2(H_2O)]_n\}$ (II), (Hökelek *et al.*, 2009), the two independent Mn^{II} atoms are located on a centre of symmetry and are coordinated by two 4-(diethylamino)benzoate (DEAB) anions and two water molecules in the basal plane, while another water molecule bridges the Mn atoms in the axial directions, forming polymeric chains as in the title compound, (I). In (II), the Mn–O bond lengths are in the range 2.1071 (14)–2.2725 (13) Å. The Mn–O bond lengths [2.2725 (13) and 2.2594 (13) Å] for the bridging water molecule are the longest with an Mn–O–Mn bond angle of 128.35 (6)°.

In the crystal structure of *catena*-[bis(μ_2 -aqua)tetraaquatetrakis(2,4,6-trimethylbenzoato-O)dinickel(II) tetrahydrate], $\{[Ni(C_{10}H_{11}O_2)_2(H_2O)_3] \cdot 2H_2O\}_n$, [(VII; Indrani *et al.*, 2009)], the two independent Ni^{II} atoms are located on a centre of symmetry and are coordinated by two 2,4,6-trimethylbenzoate (TMB) anions and two water molecules in the basal plane, while another water molecule bridges the Ni atoms in the axial directions, forming polymeric chains as in the title compound, (I). In (VII), the Ni–O bond lengths are in the range 2.0337 (15)–2.1316 (13) Å. The Ni–O bond lengths [2.1316 (13) and 2.1299 (13) Å] for the bridging water molecule are the longest with an Ni–O–Ni bond angle of 134.65 (7)°.

We also solved the crystal structure of *catena*-poly[[[diaquabis(2,4,6-trimethylbenzoato- κO^I]manganese(II)], $\{[Mn(C_{10}H_{11}O_2)_2(H_2O)_3] \cdot 2H_2O\}_n$, (VIII), which had previously been reported by Chen *et al.* (2007). In (VIII), the Mn^{II} atom and the bridging water O atom are located on a centre of symmetry and the Mn^{II} atom is coordinated by two 2,4,6-trimethylbenzoate (TMB) anions and two water molecules in the basal plane, while another water molecule

bridges the Mn^{II} cations in the axial directions, forming polymeric chains as in the title compound, (I). The Mn–O bond lengths are in the range 2.1409 (15)–2.2734 (7) Å. The Mn–O bond length [2.2734 (7) Å] for the bridging water molecule is the longest with an Mn–O–Mn bond angle of 128.41 (8)°.

In the title compound, (I), the near equalities of the C1–O1 [1.259 (4) Å] and C1–O2 [1.246 (4) Å] bonds in the carboxylate groups indicate delocalized bonding arrangements, rather than localized single and double bonds. The O2–C1–O1 bond angle [124.5 (3)°] is increased slightly compared to the free acid [122.2°] due to the coordination of oxygen atom (O1) to the metal atom. The O2–C1–O1 bond angle may be compared with the corresponding values of 121.96 (18) and 122.35 (18)° in (II), 124.0 (2)° in (III), 120.6 (6) and 121.3 (7)° in (IV), 121.7 (2) and 121.9 (3)° in (V), 123.47 (14)° in (VI), 124.29 (18) and 124.33 (18)° in (VII) and 124.02 (16)° in (VIII). The benzoate ions coordinate to the metal atoms in a monodentate fashion in (II), (III), (VI), (VII) and (VIII), and they are bidentate in (IV) and (V).

The Co1···Co1ⁱⁱ distance [4.045 (15) Å] across the chain (Fig. 2) and the Co1–O4–Co1ⁱⁱ bond angle [132.95 (13)°] in (I) may be compared with the corresponding values of 4.079 (4) Å and 128.35 (6)° in (II), 4.951 (3) Å in (III), 9.795 (4) Å in (IV), 7.363 (4) Å in (V), 4.3798 (3) Å in (VI), 3.932 Å and 134.65 (7)° in (VII) and 4.049 (15) Å and 128.41 (8)° in (VIII). According to these results, when the transition metal(II) atoms are bridged by the water molecules the $M-O_{\text{brdW}}-M$ (M = transition metal and brdW = bridging water) bond angles increase, while the $M-O_{\text{brdW}}$ bond lengths decrease with increasing atomic number, Z , of the transition metal(II) atoms and the $M \cdots M$ distances across the polymeric chains are almost the same, independent of the type of anion coordinating to the metal(II) atoms.

5. Synthesis and crystallization

The title compound was prepared by the reaction of $CoSO_4 \cdot 7H_2O$ (0.70 g, 2.5 mmol) with sodium 2,4,6-trimethylbenzoate (0.93 g, 5 mmol) in H_2O (150 ml) at room temperature. The mixture was set aside to crystallize at ambient temperature for eight weeks, giving pink single crystals (yield: 0.96 g, 81%). FT-IR: 3630, 3405, 3209, 2286, 2069, 1612, 1535, 1446, 1400, 1181, 1114, 1031, 893, 857, 827, 758, 690, 615, 570, 490, 478, 401.

6. Refinement

The experimental details including the crystal data, data collection and refinement are summarized in Table 2. H atoms of water molecules were located in difference-Fourier maps and refined with distance and angle restraints (SIMU, DELU and ISOR restraints in *SHELXL*). Bond lengths and angles for water molecules are: O3–H31 = 0.806 (19), O3–H32 = 0.818 (18), O4–H41 = 0.827 (18), O5–H51 = 0.812 (10), O5–H52 = 0.820 (10) Å and H31–O3–H32 = 107 (4) and H51–O5–H52 = 107 (4)°. The C-bound H atoms were posi-

tioned geometrically with C–H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$, where $k = 1.5$ for methyl H atoms and $k = 1.2$ for aromatic H atoms. The maximum and minimum electron densities were found 0.89 Å⁻³ and 0.82 Å⁻³ from Co1. The high residual electron density value of 2.178 e Å⁻³ may be due to the poor quality of the crystal.

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Table 2
Experimental details.

Crystal data	
Chemical formula	[Co(C ₁₀ H ₁₁ O ₂) ₂ (H ₂ O) ₃]·2H ₂ O
M_r	475.39
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	296
a, b, c (Å)	29.5261 (5), 10.1413 (2), 8.0906 (2)
β (°)	91.894 (4)
V (Å ³)	2421.27 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.75
Crystal size (mm)	0.35 × 0.29 × 0.20
Data collection	
Diffractometer	Bruker SMART BREEZE CCD diffractometer
Absorption correction	Multi-scan <i>SADABS</i> ; Bruker, 2012
$T_{\text{min}}, T_{\text{max}}$	0.779, 0.864
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25445, 2957, 2448
R_{int}	0.058
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.664
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.060, 0.166, 1.09
No. of reflections	2957
No. of parameters	161
No. of restraints	74
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)	2.18, -0.52

Computer programs: *APEX2* and *SAINTE* (Bruker, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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supporting information

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Crystal structure of *catena*-poly[[[diaquabis(2,4,6-trimethylbenzoato- κ O)cobalt(II)]- μ -aqua- κ^2 O:O] dihydrate]

Tuncer Hökelek, Nurcan Akduran, Safiye Özkaya and Hacali Necefoğlu

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINTE* (Bruker, 2012); data reduction: *SAINTE*; 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, 2012); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012) and *PLATON* (Spek, 2009).

catena-Poly[[[diaquabis(2,4,6-trimethylbenzoato- κ O)cobalt(II)]- μ -aqua- κ^2 O:O] dihydrate]

Crystal data

[Co(C₁₀H₁₁O₂)₂(H₂O)₃]·2H₂O

$M_r = 475.39$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 29.5261$ (5) Å

$b = 10.1413$ (2) Å

$c = 8.0906$ (2) Å

$\beta = 91.894$ (4)°

$V = 2421.27$ (9) Å³

$Z = 4$

$F(000) = 1004$

$D_x = 1.304$ Mg m⁻³

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

Cell parameters from 9882 reflections

$\theta = 2.8$ – 28.1 °

$\mu = 0.75$ mm⁻¹

$T = 296$ K

Block, translucent light pink

$0.35 \times 0.29 \times 0.20$ mm

Data collection

Bruker SMART BREEZE CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

SADABS; Bruker, 2012

$T_{\min} = 0.779$, $T_{\max} = 0.864$

25445 measured reflections

2957 independent reflections

2448 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\max} = 28.2$ °, $\theta_{\min} = 1.4$ °

$h = -38 \rightarrow 39$

$k = -12 \rightarrow 13$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.166$

$S = 1.09$

2957 reflections

161 parameters

74 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

$$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 9.9721P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 2.18 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.52 \text{ e } \text{\AA}^{-3}$$

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.

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.5000	0.5000	0.02399 (18)
O1	0.55057 (8)	0.6264 (2)	0.4251 (3)	0.0409 (6)
O2	0.57111 (9)	0.7216 (3)	0.6626 (3)	0.0503 (7)
O3	0.45248 (10)	0.6292 (3)	0.4084 (3)	0.0492 (7)
H31	0.4484 (17)	0.625 (6)	0.310 (2)	0.086 (17)*
H32	0.4289 (10)	0.656 (4)	0.446 (5)	0.057 (13)*
O4	0.5000	0.4132 (3)	0.2500	0.0274 (6)
H41	0.5249 (8)	0.378 (4)	0.237 (5)	0.048 (10)*
O5	0.37711 (14)	0.7250 (4)	0.5521 (4)	0.0768 (10)
H51	0.3607 (18)	0.785 (4)	0.522 (7)	0.103 (15)*
H52	0.385 (2)	0.740 (6)	0.649 (3)	0.100 (15)*
C1	0.57564 (11)	0.7012 (3)	0.5121 (4)	0.0348 (6)
C2	0.61375 (11)	0.7694 (3)	0.4254 (4)	0.0366 (7)
C3	0.65665 (13)	0.7129 (4)	0.4284 (5)	0.0509 (9)
C4	0.69080 (15)	0.7756 (5)	0.3429 (6)	0.0625 (11)
H4	0.7196	0.7386	0.3439	0.075*
C5	0.68271 (16)	0.8917 (5)	0.2564 (5)	0.0647 (12)
C6	0.64030 (15)	0.9461 (4)	0.2567 (5)	0.0567 (11)
H6	0.6349	1.0245	0.1997	0.068*
C7	0.60467 (13)	0.8874 (4)	0.3403 (4)	0.0450 (8)
C8	0.55866 (16)	0.9483 (5)	0.3372 (7)	0.0689 (12)
H8A	0.5409	0.9133	0.2458	0.103*
H8B	0.5614	1.0421	0.3252	0.103*
H8C	0.5441	0.9286	0.4387	0.103*
C9	0.7209 (2)	0.9563 (8)	0.1634 (8)	0.109 (2)
H9A	0.7152	0.9467	0.0465	0.164*
H9B	0.7491	0.9145	0.1941	0.164*
H9C	0.7225	1.0482	0.1911	0.164*
C10	0.66644 (18)	0.5874 (5)	0.5233 (7)	0.0777 (15)
H10A	0.6629	0.6028	0.6391	0.117*
H10B	0.6970	0.5597	0.5049	0.117*
H10C	0.6457	0.5198	0.4860	0.117*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0380 (3)	0.0218 (3)	0.0124 (3)	-0.00099 (18)	0.00338 (18)	-0.00010 (16)
O1	0.0549 (14)	0.0470 (13)	0.0210 (9)	-0.0202 (10)	0.0055 (9)	-0.0019 (9)
O2	0.0670 (16)	0.0616 (16)	0.0227 (10)	-0.0243 (13)	0.0073 (10)	-0.0082 (10)
O3	0.0633 (16)	0.0626 (17)	0.0221 (11)	0.0257 (13)	0.0050 (10)	0.0023 (11)
O4	0.0375 (15)	0.0275 (13)	0.0175 (12)	0.000	0.0044 (10)	0.000
O5	0.087 (2)	0.094 (3)	0.0492 (18)	0.032 (2)	-0.0007 (16)	-0.0010 (18)
C1	0.0459 (16)	0.0352 (15)	0.0234 (13)	-0.0057 (12)	0.0017 (11)	0.0016 (11)
C2	0.0439 (16)	0.0405 (16)	0.0255 (13)	-0.0142 (13)	0.0024 (11)	-0.0034 (12)
C3	0.051 (2)	0.056 (2)	0.046 (2)	-0.0079 (17)	0.0059 (15)	0.0018 (17)
C4	0.048 (2)	0.084 (3)	0.056 (2)	-0.011 (2)	0.0104 (17)	0.005 (2)
C5	0.063 (3)	0.088 (3)	0.043 (2)	-0.033 (2)	0.0041 (18)	0.011 (2)
C6	0.072 (3)	0.057 (2)	0.0398 (19)	-0.027 (2)	-0.0063 (17)	0.0137 (17)
C7	0.055 (2)	0.0468 (19)	0.0326 (16)	-0.0138 (15)	-0.0030 (14)	0.0054 (14)
C8	0.071 (3)	0.060 (3)	0.075 (3)	0.002 (2)	-0.005 (2)	0.024 (2)
C9	0.081 (4)	0.163 (6)	0.083 (4)	-0.057 (4)	0.011 (3)	0.042 (4)
C10	0.070 (3)	0.068 (3)	0.095 (4)	0.015 (2)	0.015 (3)	0.025 (3)

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

Co1—O1	2.074 (2)	C3—C10	1.509 (6)
Co1—O1 ⁱ	2.074 (2)	C4—C5	1.387 (7)
Co1—O3	2.041 (2)	C4—H4	0.9300
Co1—O3 ⁱ	2.041 (2)	C5—C9	1.524 (6)
Co1—O4	2.2060 (11)	C6—C5	1.368 (7)
Co1—O4 ⁱ	2.2060 (11)	C6—H6	0.9300
O1—C1	1.259 (4)	C7—C6	1.402 (5)
O2—C1	1.246 (4)	C7—C8	1.492 (6)
O3—H31	0.806 (19)	C8—H8A	0.9600
O3—H32	0.818 (18)	C8—H8B	0.9600
O4—Co1 ⁱⁱ	2.2060 (11)	C8—H8C	0.9600
O4—H41	0.827 (18)	C9—H9A	0.9600
O5—H51	0.812 (10)	C9—H9B	0.9600
O5—H52	0.820 (10)	C9—H9C	0.9600
C2—C1	1.513 (4)	C10—H10A	0.9600
C2—C3	1.390 (5)	C10—H10B	0.9600
C2—C7	1.401 (5)	C10—H10C	0.9600
C3—C4	1.395 (5)		
O1—Co1—O1 ⁱ	180.00 (9)	C4—C3—C10	120.5 (4)
O1—Co1—O4	87.53 (7)	C3—C4—H4	119.3
O1 ⁱ —Co1—O4	92.47 (7)	C5—C4—C3	121.5 (4)
O1—Co1—O4 ⁱ	92.47 (7)	C5—C4—H4	119.3
O1 ⁱ —Co1—O4 ⁱ	87.53 (7)	C4—C5—C9	119.7 (5)
O3—Co1—O1	89.44 (11)	C6—C5—C4	118.9 (4)
O3 ⁱ —Co1—O1	90.56 (11)	C6—C5—C9	121.4 (5)

O3—Co1—O1 ⁱ	90.56 (11)	C5—C6—C7	122.1 (4)
O3 ⁱ —Co1—O1 ⁱ	89.44 (11)	C5—C6—H6	119.0
O3 ⁱ —Co1—O3	180.00 (12)	C7—C6—H6	119.0
O3—Co1—O4	86.80 (8)	C2—C7—C6	117.7 (4)
O3 ⁱ —Co1—O4	93.20 (8)	C2—C7—C8	121.4 (3)
O3—Co1—O4 ⁱ	93.20 (8)	C6—C7—C8	120.9 (4)
O3 ⁱ —Co1—O4 ⁱ	86.80 (8)	C7—C8—H8A	109.5
O4 ⁱ —Co1—O4	180.0	C7—C8—H8B	109.5
C1—O1—Co1	128.67 (19)	C7—C8—H8C	109.5
Co1—O3—H32	131 (3)	H8A—C8—H8B	109.5
Co1—O3—H31	114 (4)	H8A—C8—H8C	109.5
H32—O3—H31	107 (4)	H8B—C8—H8C	109.5
Co1—O4—Co1 ⁱⁱ	132.95 (13)	C5—C9—H9A	109.5
Co1—O4—H41	108 (3)	C5—C9—H9B	109.5
Co1 ⁱⁱ —O4—H41	92 (3)	C5—C9—H9C	109.5
H51—O5—H52	107 (4)	H9A—C9—H9B	109.5
O1—C1—C2	116.7 (3)	H9A—C9—H9C	109.5
O2—C1—O1	124.5 (3)	H9B—C9—H9C	109.5
O2—C1—C2	118.9 (3)	C3—C10—H10A	109.5
C3—C2—C1	119.7 (3)	C3—C10—H10B	109.5
C3—C2—C7	121.3 (3)	C3—C10—H10C	109.5
C7—C2—C1	119.0 (3)	H10A—C10—H10B	109.5
C2—C3—C4	118.5 (4)	H10A—C10—H10C	109.5
C2—C3—C10	121.1 (4)	H10B—C10—H10C	109.5
O3—Co1—O1—C1	105.4 (3)	C1—C2—C3—C10	-2.7 (6)
O3 ⁱ —Co1—O1—C1	-74.6 (3)	C7—C2—C3—C4	-0.7 (6)
O4—Co1—O1—C1	-167.8 (3)	C7—C2—C3—C10	178.7 (4)
O4 ⁱ —Co1—O1—C1	12.2 (3)	C1—C2—C7—C6	-178.0 (3)
O1—Co1—O4—Co1 ⁱⁱ	-46.09 (7)	C1—C2—C7—C8	1.5 (5)
O1 ⁱ —Co1—O4—Co1 ⁱⁱ	133.91 (7)	C3—C2—C7—C6	0.6 (5)
O3—Co1—O4—Co1 ⁱⁱ	43.49 (9)	C3—C2—C7—C8	-179.9 (4)
O3 ⁱ —Co1—O4—Co1 ⁱⁱ	-136.51 (9)	C2—C3—C4—C5	0.1 (7)
Co1—O1—C1—O2	-7.3 (5)	C10—C3—C4—C5	-179.3 (5)
Co1—O1—C1—C2	172.4 (2)	C3—C4—C5—C6	0.6 (7)
C3—C2—C1—O1	-94.3 (4)	C3—C4—C5—C9	-179.5 (5)
C3—C2—C1—O2	85.4 (4)	C7—C6—C5—C4	-0.7 (7)
C7—C2—C1—O1	84.4 (4)	C7—C6—C5—C9	179.4 (5)
C7—C2—C1—O2	-95.9 (4)	C2—C7—C6—C5	0.1 (6)
C1—C2—C3—C4	177.9 (3)	C8—C7—C6—C5	-179.4 (4)

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

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

Cg1 is the centroid of the C2–C7 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H31 \cdots O1 ⁱⁱ	0.80 (2)	1.90 (2)	2.697 (3)	170 (5)

O3—H32···O5	0.82 (3)	1.91 (3)	2.724 (5)	174 (3)
O4—H41···O2 ⁱⁱⁱ	0.83 (3)	1.82 (3)	2.622 (3)	164 (4)
O5—H52···O2 ^{iv}	0.82 (3)	1.98 (4)	2.726 (4)	151 (6)
C10—H10C···O5 ⁱ	0.96	2.59	3.466 (7)	152
C6—H6···Cg1 ^v	0.93	3.28	4.063 (4)	143
C9—H9A···Cg1 ^v	0.96	3.40	3.961 (7)	120

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y, -z+1/2$; (iii) $x, -y+1, z-1/2$; (iv) $-x+1, y, -z+3/2$; (v) $-x+1/2, y+3/2, -z-1/2$.