Crystal structure of diaquasuberatocobalt(II), $\text{Co}(\text{C}_8\text{H}_{12}\text{O}_4)(\text{H}_2\text{O})_2$

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Co atom and the other bridge two Co atoms terminally. The Co atom is octahedrally coordinated by six oxygen atoms ($2\text{H}_2\text{O}$, 1 carboxyl chelate, 2 terminal bridging carboxyl with $d(\text{Co}-\text{O}) = 2.043 \text{ \AA} - 2.158 \text{ \AA}$). The C atoms and the chelating O atoms of the $\alpha,\omega\text{-OOC}(\text{CH}_2)_6\text{COO}$ dicarboxylate anion are nearly coplanar with $d(\text{C}-\text{C}) = 1.504 \text{ \AA} - 1.526 \text{ \AA}$ and $\angle(\text{C}-\text{C}-\text{C}) = 111.5^\circ - 114.1^\circ$. The second carboxyl group is twisted by about 90° ($d(\text{C}-\text{O}) = 1.257 \text{ \AA} - 1.258 \text{ \AA}$ and $\angle(\text{O}-\text{C}-\text{O}) = 118.7(3)^\circ, 120.5(3)^\circ$). One of the H_2O molecules ($d(\text{O}-\text{H}) = 0.75 \text{ \AA} - 0.84 \text{ \AA}$, $\angle(\text{H}-\text{O}-\text{H}) = 109^\circ$) forms hydrogen bonds to two carboxyl O atoms with $d(\text{O}\cdots\text{O}) = 2.721 \text{ \AA}, 2.759 \text{ \AA}$ and $\angle(\text{O}-\text{H}\cdots\text{O}) = 158.3^\circ, 173.1^\circ$, and the other to one carboxyl O atom and another crystallographically different H_2O molecule with $d(\text{O}\cdots\text{O}) = 2.811 \text{ \AA}, 2.863 \text{ \AA}$ and $\angle(\text{O}-\text{H}\cdots\text{O}) = 171.8^\circ, 162.1^\circ$.

Table 1. Data collection and handling.

Crystal:	rose-colored block, size $0.08 \times 0.12 \times 0.15 \text{ mm}$
Wavelength:	Mo K_α radiation ($0.71073 \text{ \AA}$)
μ :	16.33 cm^{-1}
Diffractometer, scan mode:	Bruker P4, $\theta/2\theta$
$2\theta_{\text{max}}$:	54.98°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	3278, 2425
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}}), 1582$
$N(\text{param})_{\text{refined}}$:	142
Programs:	SHELXS-97 [1], SHELXL-97 [2]

Abstract

$\text{C}_8\text{H}_{16}\text{CoO}_6$, monoclinic, $P12_1/c1$ (No. 14), $a = 14.856(2) \text{ \AA}$, $b = 7.449(1) \text{ \AA}$, $c = 9.614(1) \text{ \AA}$, $\beta = 97.44(1)^\circ$, $V = 1055.0 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.043$, $wR(F^2) = 0.096$, $T = 293 \text{ K}$.

Source of material

The title compound was synthesized by the reaction of 0.5 g (2.90 mmol) suberic acid with an excess of fresh CoCO_3 in 25 ml twice-distilled water, followed by filtrating the unreacted CoCO_3 . The filtrate was then maintained at 331 K and rose-colored crystals formed within two days.

Discussion

The crystal structure consists of ${}_2[\text{Co}(\text{H}_2\text{O})_2(\text{C}_8\text{H}_{12}\text{O}_4)_{3/3}]$ layers with H_2O molecules between. $\alpha,\omega\text{-OOC}(\text{CH}_2)_6\text{COO}$ zig-zag chains parallel to $[100]$ are fragments of the 2D layers which extend parallel to (100) and are held together by hydrogen bonds. Each $\alpha,\omega\text{-OOC}(\text{CH}_2)_6\text{COO}$ dicarboxylate anion links three Co atoms. One terminal carboxyl group acts as chelate ligand to one

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{iso}
Ha(O5)	4e	0.5296	0.2041	0.5340	0.05(1)
Hb(O5)	4e	0.6191	0.2284	0.5260	0.10(2)
Ha(O6)	4e	0.4472	0.0895	0.7282	0.06(2)
Hb(O6)	4e	0.4575	-0.0573	0.7912	0.06(2)
H(2A)	4e	0.7296	-0.4674	0.5696	0.047(3)
H(2B)	4e	0.7296	-0.3109	0.6788	0.047(3)
H(3A)	4e	0.8186	-0.2974	0.4354	0.047(3)
H(3B)	4e	0.8137	-0.1318	0.5348	0.047(3)
H(4A)	4e	0.8976	-0.2981	0.7196	0.047(3)
H(4B)	4e	0.9066	-0.4552	0.6139	0.047(3)
H(5A)	4e	0.9892	-0.2577	0.4818	0.047(3)
H(5B)	4e	0.9863	-0.1127	0.5991	0.047(3)
H(6A)	4e	1.0765	-0.4447	0.6432	0.047(3)
H(6B)	4e	1.0743	-0.2981	0.7594	0.047(3)
H(7A)	4e	1.1570	-0.2356	0.5157	0.047(3)
H(7B)	4e	1.1631	-0.1074	0.6457	0.047(3)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Co	4e	0.61398(3)	0.01039(7)	0.72373(4)	0.0309(2)	0.0407(3)	0.0274(2)	−0.0010(2)	0.0045(2)	−0.0015(2)
O(1)	4e	0.6284(2)	−0.2934(3)	0.3671(2)	0.041(1)	0.047(1)	0.026(1)	0.003(1)	0.001(1)	−0.006(1)
O(2)	4e	0.5937(2)	−0.1607(4)	0.5560(2)	0.034(1)	0.050(2)	0.032(1)	0.004(1)	0.002(1)	−0.009(1)
O(3)	4e	1.3206(2)	−0.2939(4)	0.6315(3)	0.036(1)	0.058(2)	0.038(1)	0.003(1)	0.009(1)	0.009(1)
O(4)	4e	1.2463(2)	−0.4339(4)	0.7788(3)	0.034(1)	0.059(2)	0.045(2)	0.002(1)	0.007(1)	0.016(1)
O(5)	4e	0.5784(2)	0.2269(3)	0.5795(3)	0.035(1)	0.046(2)	0.033(1)	−0.002(1)	0.003(1)	−0.001(1)
O(6)	4e	0.4823(2)	0.0199(4)	0.7637(3)	0.035(1)	0.052(2)	0.060(2)	0.005(1)	0.012(1)	0.016(2)
C(1)	4e	0.6454(2)	−0.2603(5)	0.4966(3)	0.034(2)	0.034(2)	0.032(2)	−0.007(1)	0.003(1)	−0.000(2)
C(2)	4e	0.7299(2)	−0.3379(5)	0.5802(4)	0.034(2)	0.047(2)	0.032(2)	0.004(2)	0.004(1)	−0.002(2)
C(3)	4e	0.8161(2)	−0.2619(5)	0.5319(4)	0.034(2)	0.048(2)	0.038(2)	0.004(2)	0.005(2)	0.001(2)
C(4)	4e	0.9021(2)	−0.3259(6)	0.6222(4)	0.034(2)	0.057(2)	0.040(2)	0.004(2)	0.004(2)	0.002(2)
C(5)	4e	0.9882(2)	−0.2409(6)	0.5816(4)	0.038(2)	0.055(2)	0.043(2)	0.004(2)	0.004(2)	0.007(2)
C(6)	4e	1.0749(2)	−0.3164(6)	0.6597(4)	0.035(2)	0.053(2)	0.043(2)	0.002(2)	0.005(2)	0.005(2)
C(7)	4e	1.1605(2)	−0.2324(5)	0.6171(4)	0.035(2)	0.044(2)	0.048(2)	0.004(2)	0.007(2)	0.004(2)
C(8)	4e	1.2465(2)	−0.3240(5)	0.6795(4)	0.036(2)	0.040(2)	0.033(2)	0.000(2)	0.004(1)	−0.003(2)

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