Crystal structure of *catena*-poly[mono(μ -aqua)di(μ -acetato)cobalt(II)] monohydrate, $[\text{Co}(\text{CH}_3\text{COO})_2(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$

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Abstract

$\text{C}_4\text{H}_{10}\text{CoO}_6$, monoclinic, $P12_1/c1$ (No. 14), $a = 8.9948(6)$ Å, $b = 6.4157(4)$ Å, $c = 13.7402(9)$ Å, $\beta = 108.539(1)^\circ$, $V = 751.8$ Å³, $Z = 4$, $R_{\text{int}}(F) = 0.023$, $wR(F^2) = 0.066$, $T = 173$ K.

Source of material

Pink crystals of the title compound were grown over several months from 10 ml of a $0.12 \text{ mol} \cdot \text{l}^{-1}$ $\text{Co}(\text{OAc})_2(\text{H}_2\text{O})_4$ acetic acid solution.

Discussion

Cobalt acetate is the most widely used homogenous catalyst in industry [1–3]. From the structural point of view, acetate is an important organic ligand, which exhibits various coordination modes observed in by $[\text{Co}_4(\mu_3\text{O})_4(\mu\text{-CH}_3\text{COO})_4(\text{C}_5\text{H}_5\text{N})_4]\text{CHCl}_3$ [4], $\text{Pb}(\text{CH}_3\text{COO})\text{L}(\text{BPh}_4)$ ($\text{L} = 1,4,7\text{-triazacyclononane}$) [5], $[\text{Ag}_2(4\text{-hmt})(\mu\text{-CH}_3\text{COO})]\text{CH}_3\text{COO} \cdot 4.5\text{H}_2\text{O}$ ($\text{hmt} = \text{hexamethylethylenetetraamine}$), [6], $[\text{Re}(\text{CO})_3(\mu\text{-CH}_3\text{COO})\text{THF}]_4$ [7], $[\text{PPh}_4]_2[\text{Ru}_2\text{O}(\mu\text{-CH}_3\text{COO})_2\text{Cl}_6]$ [8].

Here we report an infinite-chain cobalt acetate compound $[\text{Co}(\text{OAc})_2\text{H}_2\text{O} \cdot \text{H}_2\text{O}]_n$. The chains are formed by cobalt(II) cations linked with bridging acetate groups and water molecules. The linear chains in turn are connected to each other by a network of hydrogen bonds to solvate water molecules. The cobalt atom possesses a severely distorted octahedral geometry with the *cis*-angles about the Co atom ranging from $77.95(5)^\circ$ – $110.34(5)^\circ$. The Co—O(acetate) distances vary between $2.0401(13)$ Å – $2.1002(13)$ Å while the Co—O(water) bond length measured $2.1595(13)$ Å and $2.2088(13)$ Å. These distances fall in the usual ranges for Co—O bond distances to bridging lig-

ands. There are two types of bridging acetate groups in the complex. One acetate coordinates with each of its oxygen atoms to a different Co atom and its C—O lengths are equivalent. The other acetate group links two cobalt atoms with one μ -O atom, hence the C—O distances in this ligand are distinctly different. There are three likely hydrogen bonding interactions in the lattice that link the polymeric linear chains. These hydrogen bonds are formed between the coordinate and solvate water molecules. The corresponding values for O...O separations and H—O—H angles are as follows: O(5)—H(5a)...O(6) 2.606 Å and 160° ; O(6)—H(6a)...O(4) [$x-1, -y, 2-z$] 2.721 Å and 177° and O(6)—H(6b)...O(3) [$x-1, 1-y, 2-z$] 2.768 Å and 175° . It is noteworthy that the crystal structure of $[\text{Co}(\text{OAc})_2(\text{H}_2\text{O}) \cdot \text{H}_2\text{O}]_n$ is quite different from that of $\text{Co}(\text{OAc})_2(\text{H}_2\text{O})_4$ recrystallized from water [9,10] in which four water molecules are coordinated to Co(II) and $\text{Co}(\text{OAc})_2$ (dehydrated) [11]. In acetic acid, cobalt(II) acetate forms a dimeric complex similar to $[\text{Co}(\text{OAc})_2\text{H}_2\text{O} \cdot \text{H}_2\text{O}]_n$ except for its polymeric structure and water molecules coordinated to Co(II).

Table 1. Data collection and handling.

Crystal:	pink block, size $0.10 \times 0.30 \times 0.50$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	22.65 cm^{-1}
Diffractometer, scan mode:	Bruker CCD, ω
$2\theta_{\text{max}}$:	52.74°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	1539, 1539
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1444
$N(\text{param})_{\text{refined}}$:	111
Programs:	SHELXS-97 [12], SHELXL-97 [13]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U _{iso}
H(5A)	4e	0.3687	0.4913	0.8602	0.017
H(5B)	4e	0.2527	0.5003	0.7424	0.017
H(6A)	4e	0.334(3)	0.410(3)	1.005(2)	0.031(7)
H(6B)	4e	0.351(3)	0.618(3)	1.003(2)	0.038(8)
H(1A)	4e	-0.0199	0.0501	0.6142	0.039

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(1B)	4e	0.1240	0.1980	0.6157	0.039
H(1C)	4e	0.0745	0.1715	0.7171	0.039
H(3A)	4e	0.8356	0.1127	1.0526	0.034
H(3B)	4e	0.8227	-0.1344	1.0638	0.034
H(3C)	4e	0.7097	0.0176	1.1004	0.034

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(1)	4e	0.48429(3)	0.22719(4)	0.74898(2)	0.0138(2)	0.0090(2)	0.0102(2)	0.00009(8)	0.0021(1)	0.00001(8)
O(1)	4e	0.3435(2)	-0.0400(2)	0.7260(1)	0.0132(6)	0.0117(6)	0.0147(7)	0.0009(5)	0.0021(5)	0.0001(5)
O(2)	4e	0.1423(2)	-0.2614(2)	0.6802(1)	0.0168(7)	0.0169(8)	0.0295(8)	-0.0027(5)	0.0024(6)	0.0024(5)
O(3)	4e	0.5799(2)	0.1540(2)	0.90319(9)	0.0214(7)	0.0126(7)	0.0125(6)	0.0009(5)	0.0031(5)	-0.0003(5)
O(4)	4e	0.6155(2)	-0.1902(2)	0.9011(1)	0.0256(7)	0.0121(7)	0.0126(6)	-0.0003(5)	0.0021(5)	-0.0001(5)
O(5)	4e	0.3632(2)	0.4899(2)	0.7871(1)	0.0154(6)	0.0132(6)	0.0129(7)	0.0004(5)	0.0040(5)	-0.0006(5)
O(6)	4e	0.3153(2)	0.5140(2)	0.9640(1)	0.0256(8)	0.0143(7)	0.0136(7)	0.0002(5)	0.0040(6)	0.0009(5)
C(1)	4e	0.0835(2)	0.1004(3)	0.6560(2)	0.0155(9)	0.020(1)	0.037(1)	0.0033(8)	0.0026(9)	0.0027(9)
C(2)	4e	0.1941(2)	-0.0813(3)	0.6885(1)	0.0153(9)	0.0157(9)	0.0145(8)	-0.0003(7)	0.0037(7)	0.0010(7)
C(3)	4e	0.7635(3)	-0.0035(3)	1.0494(2)	0.026(1)	0.018(1)	0.017(1)	0.0002(8)	-0.0027(9)	-0.0011(7)
C(4)	4e	0.6444(2)	-0.0134(3)	0.9438(2)	0.0164(9)	0.0130(9)	0.0125(9)	-0.0014(7)	0.0055(7)	0.0002(6)

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