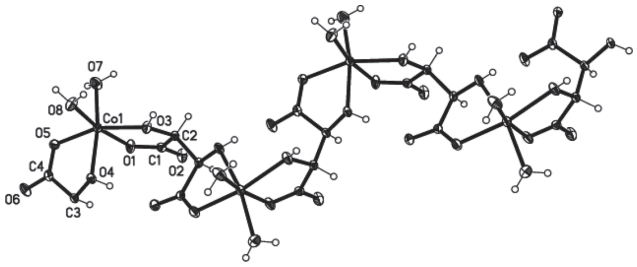
Sisi Feng, Haixia Ma and Miaoli Zhu*

Crystal structure of *catena*-poly[diaqua-(μ_2-tartrato-$\kappa^4O,O':O'',O'''$)cobalt(II)], $C_4H_8CoO_8$



https://doi.org/10.1515/ncrs-2017-0214
Received September 11, 2017; accepted November 25, 2017; available online December 14, 2017

Abstract

$C_4H_8CoO_8$, monoclinic, $P2_1/c$ (no. 14), $a = 5.7952(3)$ Å, $b = 13.0110(7)$ Å, $c = 10.2682(6)$ Å, $\beta = 98.8320(10)°$, $V = 765.06(7)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0207$, $\omega R_{ref}(F^2) = 0.0499$, $T = 301(2)$ K.

CCDC no.: 1563530

A part of the chain-type title structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

$Co(CH_3COO)_2{\cdot}4H_2O$ (0.072 mmol) and oxirane-2,3-dicarboxylic acid (0.072 mmol) were dissolved in water (4.0 mL), mixed and left at 301 K in a tube. Violet block crystals of the title compound appeared after 1 week in 30% yield.

Experimental details

Hydrogen atoms attached to C atoms were placed geometrically and refined using a riding model approximation, with C—H = 0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Hydrogen atoms attached to O atoms were located from difference Fourier maps and refined using their global U_{iso} value.

Table 1: Data collection and handling.

Crystal:	Block, violet
Size:	0.30 × 0.20 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.26 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7058, 1764, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1708
$N(param)_{refined}$:	151
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
Co1	0.16895(3)	0.41271(2)	0.71120(2)	0.01285(9)
C1	0.5423(2)	0.38251(11)	0.93314(14)	0.0136(3)
C2	0.3294(2)	0.35752(11)	0.99918(13)	0.0122(3)
H2	0.325(3)	0.4105(14)	1.063(2)	0.017(5)*
C3	0.3637(2)	0.24470(10)	0.57264(13)	0.0125(3)
H3	0.511(3)	0.2443(14)	0.6191(18)	0.016(4)*
C4	0.3509(2)	0.33943(11)	0.48294(13)	0.0141(3)
O1	0.50824(18)	0.40583(9)	0.81246(11)	0.0191(2)
O2	0.73633(18)	0.38243(10)	1.00502(11)	0.0211(2)
O3	0.12522(18)	0.35939(9)	0.90261(10)	0.0164(2)
H3A	0.019(4)	0.3680(19)	0.937(2)	0.038(6)*
O4	0.19539(19)	0.25550(8)	0.66020(10)	0.0167(2)
H4	0.246(4)	0.2275(17)	0.724(2)	0.028(6)*
O5	0.2717(2)	0.42064(8)	0.52643(11)	0.0182(2)
O6	0.4294(2)	0.33164(9)	0.37686(10)	0.0216(2)
O7	0.1916(2)	0.57357(9)	0.72712(13)	0.0244(3)
H7A	0.201(5)	0.5928(19)	0.801(3)	0.042(7)*
H7B	0.286(5)	0.600(2)	0.685(3)	0.048(8)*
O8	−0.1760(2)	0.42309(9)	0.64623(12)	0.0212(2)
H8A	−0.211(4)	0.476(2)	0.595(3)	0.039(6)*
H8B	−0.258(5)	0.4218(19)	0.701(3)	0.043(7)*

Discussion

Hydroxypolycarboxylic acids can act as hydrogen–bond acceptors and donors simultaneously, depending on the number of deprotonated carboxyl group. In all known tartrate-bridging complexes, the oxygen atoms of the alkoxyl

***Corresponding author: Miaoli Zhu,** Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular Engineering of the Education Ministry, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China, e-mail: miaoli@sxu.edu.cn
Sisi Feng and Haixia Ma: Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular Engineering of the Education Ministry, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China

or hydroxyl groups participate in the coordination process, which allows the formation of five- and six-membered rings, stabilizing the network in the solid state [3]. We have recently studied the assembly reactions of oxirane-2,3-dicarboxylic acid with transition metal ions and obtained a Co(II) complex based on the *in situ* generated tartrate ligand. Herein, we report the one-dimensional structure, namely $[Co(H_4tar)(H_2O)_2]_n$ (H_4tar = tartrate dianion).

The asymmetric unit of the title complex, $[Co(C_4H_4O_6)(H_2O)_2]$, consists of one Co(II) cation, one double deprotonated tartrate anion and two coordinated water molecules. The coordination geometry of the Co(II) cation is a distorted octahedron with two O atoms from two coordinated water molecules occupying *cis* positions in the equatorial plane and four O atoms from two tartrate ligands occupying the remaining positions. The bond lengths of Co-O range from 2.0128(13) to 2.1400(12) Å, which are similar to those found in other transition-metal complexes of tartrate [4, 5]. The angles of O-Co1-O range from 76.37(5) to 169.48(5)°, which indicates that the Co center exhibits a significantly distorted octahedral geometry. The structure is isotypic to the Mg compound $[Mg(meso\text{-}C_4H_4O_6)(H_2O)_2]$ [6] with the similar coordination configuration, bond lengths and angles except for the metal cation. Compared with similar structures [7–9], the title complex is not forming the dinuclear unit but forms a chain along the *c* direction. Moreover, the complex crystallizes in the centrosymmetric space group $P2_1/c$ rather than the chiral one, which probably because the tartrate is generated by the decomposition of oxirane-2,3-dicarboxylic acid. The tartrate ion coordinates to Co center *via* an undeprotonated hydroxyl group and one monodentate carboxylate group (*cf*. the figure). The ligand connects two Co centers by a bidentate-bridging coordination. Thus, adjacent Co centers show a separation of 6.655 Å. In the crystal, intermolecular O—H···O hydrogen bonds involving the carboxylate oxygen atoms and lattice water molecules link the molecules into a three-dimensional network.

Acknowledgements: This work was supported by the Natural Science Foundation of China (Grant Nos 21201113 & 21671124) and the Scientific Instrument Center of Shanxi University of China.

References

1. Bruker: APEX2, SAINT and SADABS. Brucker AXS Inc., Madison, WI, USA (2009).
2. Sheldrick, G. M.: Crystal structure refi nement with SHELXL. Acta Crystallogr. **C71** (2015) 3–8.
3. Gu, Y. B.; Yang, M. H.: Synthesis, characterization of an unusual crystalline material with tartrate. Cryst. Res. Technol. **43** (2008) 1331–1334.
4. Li, D. X.; Xu, D. J.; Xu, Y. Z.: Catena-Poly[[[diaquacobalt(II)]-μ-tartrato-K^4*O,O′:O″,O‴*] monohydrate]. Acta Crystallogr. E **60** (2004) 1982–1984.
5. Du, C. J.; Zhang, L. S.; Du, C. L.: Diaquabis(hydrogen tartrato) cobalt(II) dehydrate. Acta Crystallogr. E **68** (2012) 99–100.
6. Kam, K. C.; Young, K. L. M.; Cheetham, A. K.: Chemical and structural diversity in chiral magnesium tartrates and their racemic and meso analogues. Cryst. Growth Des. **7** (2007) 1522–1532.
7. Wicharz, R.; Wartchow, R.; Jaeckel, M.: Crystal structure of bis[aqua-μ-(2*R*,3*R*)-tartratocobalt(II)] trihydrate, $[\{Co(C_4H_4O_6)(H_2O)\}_2]\cdot 3H_2O$. Z. Kristallogr. NCS. **212** (1997) 81–82.
8. Belombe, M. M.; Nenwa, J.; Fokwa, B. P. T.; Dronskowski, R.: Crystal structure of catena-bis[aqua-μ-(2*S*,3*S*)-tartratocobalt (II)] trihydrate, $[Co(H_2O)(C_4H_4O_6)]_2\cdot 3H_2O$, a new polymorph. Z. Kristallogr. NCS. **224** (2009) 241–242.
9. Coronado, E.; Galan-Mascaros, J. R.; Gomez-Garcia, C. J.; Murcia-Martinez, A.: Chiral molecular magnets: synthesis, structure, and magnetic behavior of the series [M-(L-tart)] (M = Mn_{II}, Fe_{II}, Co_{II}, Ni_{II}; L-tart = (2*R*,3*R*)-(+)-tartrate). Chem-Eur J. **12** (2006) 3484–3492.