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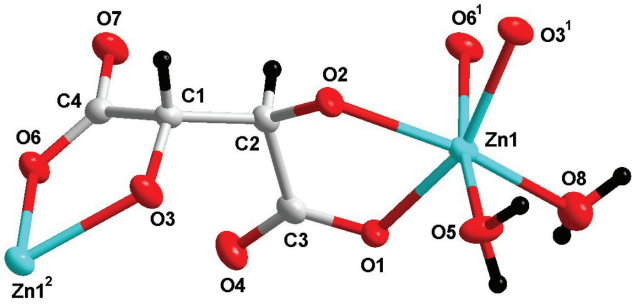
# Crystal structure of *catena*-poly[diaqua-($\mu_2$-tartrato-$\kappa^4O,O':O'',O'''$)zinc(II)], $C_4H_8O_8Zn$

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## Abstract

$C_4H_8O_8Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 5.8031(2)$ Å, $b = 13.0103(4)$ Å, $c = 10.2425(3)$ Å, $\beta = 98.954(3)°$, $V = 763.89(4)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0330$, $wR_{ref}(F^2) = 0.0784$, $T = 293(2)$ K.

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A part of the title coordination polymer structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

## Source of material

Racemic tartaric acid (0.030 g, 0.2 mmol) was added to 10 mL bidestilled water under stirring. After 15 min, it became a clear solution. To the solution $Zn(OAc)_2 \cdot 4H_2O$ (0.044 g, 0.2 mmol) was added drop by drop. The pH was adjusted to 5.5 with 1 M NaOH solution. The solution was stirred for another 15 min, then filtered. The filtrate was let evaporate in air. Several weeks later, colorless crystals were obtained, yield 56% (based on racemic tartaric acid).

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.23 × 0.21 × 0.16 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 3.23 mm$^{-1}$ |
| Diffractometer, scan mode: | Xcalibur, $\omega$ |
| $\theta_{max}$, completeness: | 28.9°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 3499, 1750, 0.027 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 1473 |
| $N(param)_{refined}$: | 128 |
| Programs: | CrysAlis$^{PRO}$ [1], Olex2 [2], SHELX [3, 4] |

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

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.16670(6) | 0.58428(3) | 0.70926(3) | 0.01917(13) |
| O1 | 0.2712(4) | 0.57946(15) | 0.5273(2) | 0.0214(5) |
| O2 | 0.1870(4) | 0.74507(18) | 0.6572(2) | 0.0233(5) |
| O3 | 0.1234(4) | 0.86053(18) | 0.4015(2) | 0.0220(5) |
| O4 | 0.4275(4) | 0.66848(17) | 0.3781(2) | 0.0286(5) |
| O5 | −0.1768(4) | 0.57579(16) | 0.6501(2) | 0.0269(5) |
| H5A | −0.208643 | 0.523329 | 0.599199 | 0.040* |
| H5B | −0.264853 | 0.577169 | 0.717619 | 0.040* |
| O6 | 0.5051(4) | 0.90573(16) | 0.3127(2) | 0.0236(5) |
| O7 | 0.7333(4) | 0.88097(18) | 0.5054(2) | 0.0270(5) |
| O8 | 0.1929(4) | 0.42381(16) | 0.7243(2) | 0.0324(6) |
| H8A | 0.208000 | 0.404386 | 0.804509 | 0.049* |
| H8B | 0.307672 | 0.392846 | 0.675700 | 0.049* |
| C1 | 0.3261(5) | 0.8575(2) | 0.4983(3) | 0.0173(6) |
| H1 | 0.311603 | 0.911688 | 0.562945 | 0.021* |
| C2 | 0.3582(5) | 0.7562(2) | 0.5723(3) | 0.0188(6) |
| H2A | 0.511762 | 0.757568 | 0.627897 | 0.023* |
| C3 | 0.3491(5) | 0.6613(2) | 0.4834(3) | 0.0199(6) |
| C4 | 0.5401(5) | 0.8823(2) | 0.4331(3) | 0.0195(6) |
| H2 | 0.227(6) | 0.773(3) | 0.719(3) | 0.019(10)* |
| H3 | 0.015(6) | 0.869(3) | 0.433(4) | 0.024(10)* |

## Experimental details

The structure was solved by direct methods with the SHELXS program. All H-atoms from C atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.98 Å ($U_{iso}(H) = 1.2U_{eq}(C)$) and with O—H = 0.87 Å ($U_{iso}(H) = 1.5U_{eq}(O)$), respectively. The H2 and H3 atoms from O atoms were located based on difference electron peaks.

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## Comment

Tartrate is a useful ligand to construct metal-organic framewoks. Many coodination compounds based on Zn(II) and tartaric acid have been reported [5–9]. Some N-containing co-ligands such as imidazole, triazole, 1,3-propanediyl)bis(1*H*-benzimidazole and 1,10-phenanthroline were used to construct the corresponding coordination polmers [10–13]. We herein report one crystal structure of Zn(II) complex based on racemic tartaric acid.

The asymmetric unit is made of one $\mu_2$-tartrate, one Zn(II) cation, and two water molecules. As shown in the figure, the Zn(II) is hexa-coordinated with four O atoms from the $\mu_2$-tartrate and two coordinated water molecules. The tetra-dentate tartrate acts as bridging ligand to link two Zn(II) to generate the one-dimensional title structure, comparable with the literature [14]. A three-dimensional structure is formed through hydrogen bonds: O2—H2···O4, O3—H3···O7, O5—H5A···O1, O5—H5B···O6, O8—H8A···O7 and O8—H8B···O4. All the bond lengths of the title compound are comparable with its analogues [5–14].

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