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# Poly[[diaqua-$\mu_4$-tartrato-$\mu_2$-tartrato-dimanganese(II)] dihydrate]

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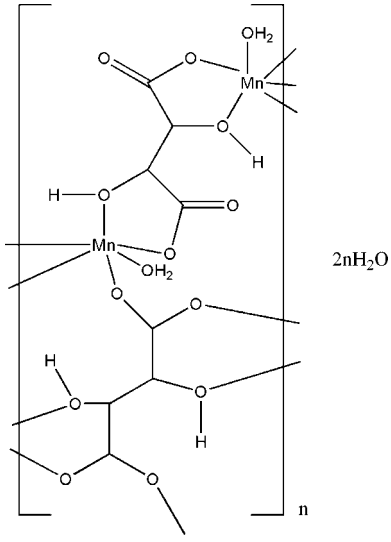
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.028; $wR$ factor = 0.074; data-to-parameter ratio = 12.8.

In the title compound, $\{[Mn(C_4H_4O_6)(H_2O)]\cdot H_2O\}_n$, the $Mn^{2+}$ ion is connected to three different tartrate anions and a water molecule, resulting in a distorted $MnO_6$ octahedral geometry. There are two tartrate half-anions in the asymmetric unit, both of which are completed by crystallographic twofold rotation symmetry. The tartrate dianions bridge the $Mn^{2+}$ ions to form a wave-like infinite layer. A series of O—H···O hydrogen bonds link the layers into a three-dimensional network.

## Related literature

For related literature, see: Kam *et al.* (2007).




## Experimental

### Crystal data

$[Mn(C_4H_4O_6)(H_2O)]\cdot H_2O$
$M_r$ = 239.04
Monoclinic, $P2_1/c$
$a$ = 11.029 (3) Å
$b$ = 7.3925 (18) Å
$c$ = 10.165 (3) Å
$\beta$ = 112.149 (3)°
$V$ = 767.6 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.74 mm$^{-1}$
$T$ = 293 (2) K
0.25 × 0.20 × 0.18 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.661, $T_{max}$ = 0.739
3884 measured reflections
1507 independent reflections
1481 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.012

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.074
$S$ = 1.10
1507 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.69 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Mn1—O6 | 2.1036 (15) | Mn1—O1*W* | 2.2018 (16) |
| Mn1—O1 | 2.1444 (15) | Mn1—O3 | 2.2230 (14) |
| Mn1—O5$^{i}$ | 2.1695 (15) | Mn1—O4$^{i}$ | 2.2518 (14) |

Symmetry code: (i) $x, -y, z-\frac{1}{2}$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···O2*W*$^{ii}$ | 0.82 | 1.81 | 2.628 (2) | 175 |
| O3—H3*A*···O2$^{iii}$ | 0.82 | 1.75 | 2.561 (2) | 173 |
| O1*W*—H1*WA*···O2$^{iv}$ | 0.82 | 2.04 | 2.643 (2) | 130 |
| O2*W*—H2*WA*···O5$^{v}$ | 0.82 | 2.29 | 2.895 (2) | 131 |
| O2*W*—H2*WB*···O4$^{i}$ | 0.82 | 2.25 | 2.919 (3) | 140 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

This project was supported by the Natural Science Foundation of the Education Bureau of Liaoning Province (grant No. 05 L159).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2676).

## References

Bruker (2001). *SMART* (Version 5.624), *SAINT* (Version 6.04) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Kam, K. C., Young, K. L. M. & Cheetham, A. K. (2007). *Cryst. Growth Des.* **7**, 1522–1532.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. University of Göttingen, Germany.

# supplementary materials

*Acta Cryst.* (2008). E**64**, m360 [ **doi:10.1107/S1600536807067839** ]

# Poly[[diaqua-$\mu_4$-tartrato-$\mu_2$-tartrato-dimanganese(II)] dihydrate]

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## Comment

Researchers have been interested in the study of tartrate-based coordination polymers, which has resulted in the formation of many interesting structures (*e.g.* Kam *et al.*, 2007). The title compound, (I), is centrosymmetric (Fig. 1). The Mn(II) ion adopts a distorted $MnO_6$ octahedral geometry (Table 1).

In the crystal, one (*R,R*) and one (*S,S*) tartrate ligands coordinate with two metal ions to form a 'tetrameric' A ring (Fig. 2). Then, two (*R,R*), two (*S,S*) tartrate ligands and four metal ions form 'hexameric' B ring (Fig. 2). Overal, a layered, two-dimensional, coordination polymer arises. The layers encompass small channels occupied by the uncoordinated water molecules, which interact with the layers by way of O—H···O hydrogen bonds (Table 2).

## Experimental

A mixture of aqueous $Mn(NO_3)_2$ (2 mmol), racemic tartaric acid (2 mmol) and NaOH (4 mmol) in 20 ml water was stirred for 2 h. The resulting solution was filtered and allowed to stand in air. Slow evaporation at room temperature for several weeks yielded yellow blocks of (I).

## Refinement

The H atoms were located in a different map, relocated in idealized positions (C—H = 0.98 Å, O—H = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

## Figures

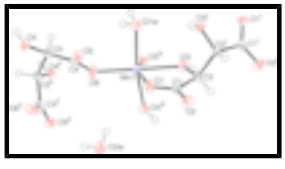

Fig. 1. View of (I), showing displacement ellipsoids drawn at 50% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i) -*x*, *y*, 1/2 - *z*; (ii) 1 - *x*, *y*, 3/2 - *z*; (iii) *x*, -*y*, *z* - 1/2.

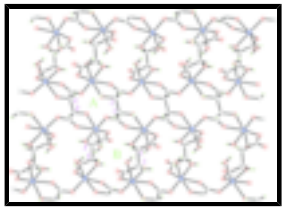

Fig. 2. View of the layered network in (I) along [010] direction, with the A and B rings indicated (see text).

**Poly[[diaqua-μ$_4$-tartrato-μ$_2$-tartrato-dimanganese(II)] dihydrate]**

*Crystal data*

| | |
|---|---|
| $[Mn(C_4H_4O_6)(H_2O)]\cdot H_2O$ | $F_{000}$ = 484 |
| $M_r$ = 239.04 | $D_x$ = 2.068 Mg m$^{-3}$ |
| Monoclinic, *P*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yc | Cell parameters from 456 reflections |
| *a* = 11.029 (3) Å | θ = 2.8–22.3º |
| *b* = 7.3925 (18) Å | μ = 1.74 mm$^{-1}$ |
| *c* = 10.165 (3) Å | *T* = 293 (2) K |
| β = 112.149 (3)º | Block, yellow |
| *V* = 767.6 (3) Å$^3$ | 0.25 × 0.20 × 0.18 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 1507 independent reflections |
| Radiation source: fine-focus sealed tube | 1481 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.012 |
| *T* = 293(2) K | $\theta_{max}$ = 26.0º |
| ω scans | $\theta_{min}$ = 2.0º |
| Absorption correction: multi-scan (SADABS; Bruker, 2001) | *h* = −12→13 |
| $T_{min}$ = 0.661, $T_{max}$ = 0.739 | *k* = −9→5 |
| 3884 measured reflections | *l* = −12→12 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.027 | H-atom parameters constrained |
| $wR(F^2)$ = 0.074 | $w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.6888P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.11 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1507 reflections | $\Delta\rho_{max}$ = 0.45 e Å$^{-3}$ |
| 118 parameters | $\Delta\rho_{min}$ = −0.69 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mn1 | 0.25422 (3) | 0.14754 (4) | 0.41123 (3) | 0.01934 (13) |
| C1 | 0.13897 (18) | 0.5035 (3) | 0.43625 (19) | 0.0179 (4) |
| C2 | 0.07525 (17) | 0.4815 (2) | 0.27492 (18) | 0.0162 (4) |
| H2 | 0.1024 | 0.5821 | 0.2294 | 0.019* |
| C3 | 0.42697 (17) | −0.2562 (3) | 0.74009 (19) | 0.0181 (4) |
| H3 | 0.3829 | −0.3503 | 0.6706 | 0.022* |
| C4 | 0.35823 (17) | −0.0765 (3) | 0.68319 (19) | 0.0200 (4) |
| O1 | 0.20895 (14) | 0.3801 (2) | 0.51027 (14) | 0.0251 (3) |
| O2 | 0.11465 (16) | 0.65022 (18) | 0.48441 (15) | 0.0242 (3) |
| O3 | 0.11895 (14) | 0.31700 (19) | 0.23691 (14) | 0.0212 (3) |
| H3A | 0.1245 | 0.3256 | 0.1590 | 0.032* |
| O4 | 0.41270 (13) | −0.30125 (19) | 0.87015 (14) | 0.0206 (3) |
| H4 | 0.4041 | −0.4114 | 0.8703 | 0.031* |
| O5 | 0.28552 (14) | −0.00821 (19) | 0.73884 (15) | 0.0241 (3) |
| O6 | 0.37862 (15) | −0.0127 (2) | 0.57879 (16) | 0.0315 (4) |
| O1W | 0.08037 (15) | −0.0100 (2) | 0.39729 (17) | 0.0306 (3) |
| H1WA | 0.0662 | −0.1156 | 0.3707 | 0.046* |
| H1WB | 0.0915 | −0.0298 | 0.4808 | 0.046* |
| O2W | 0.6263 (2) | 0.3474 (2) | 0.6453 (2) | 0.0511 (5) |
| H2WA | 0.6577 | 0.2909 | 0.7200 | 0.077* |
| H2WB | 0.5735 | 0.2819 | 0.5859 | 0.077* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mn1 | 0.02154 (19) | 0.01935 (19) | 0.01749 (19) | 0.00330 (10) | 0.00775 (13) | 0.00311 (10) |
| C1 | 0.0182 (8) | 0.0198 (9) | 0.0160 (9) | −0.0034 (7) | 0.0067 (7) | −0.0012 (7) |
| C2 | 0.0180 (9) | 0.0170 (9) | 0.0139 (8) | 0.0015 (7) | 0.0064 (7) | 0.0005 (7) |
| C3 | 0.0175 (9) | 0.0200 (9) | 0.0165 (8) | −0.0014 (7) | 0.0060 (7) | 0.0010 (7) |
| C4 | 0.0158 (8) | 0.0228 (10) | 0.0182 (9) | −0.0014 (7) | 0.0028 (7) | 0.0040 (7) |
| O1 | 0.0303 (8) | 0.0254 (7) | 0.0158 (7) | 0.0064 (6) | 0.0045 (6) | 0.0005 (5) |
| O2 | 0.0358 (8) | 0.0200 (7) | 0.0177 (7) | 0.0007 (6) | 0.0110 (6) | −0.0020 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.0274 (7) | 0.0235 (7) | 0.0143 (6) | 0.0079 (6) | 0.0095 (5) | 0.0012 (5) |
| O4 | 0.0242 (7) | 0.0193 (7) | 0.0208 (7) | 0.0014 (5) | 0.0112 (5) | 0.0051 (5) |
| O5 | 0.0274 (7) | 0.0215 (7) | 0.0261 (7) | 0.0038 (6) | 0.0131 (6) | 0.0038 (5) |
| O6 | 0.0261 (7) | 0.0416 (9) | 0.0294 (8) | 0.0111 (6) | 0.0136 (6) | 0.0194 (7) |
| O1W | 0.0302 (8) | 0.0250 (8) | 0.0336 (8) | −0.0013 (6) | 0.0086 (6) | 0.0057 (6) |
| O2W | 0.0643 (13) | 0.0254 (9) | 0.0473 (12) | 0.0007 (8) | 0.0024 (10) | 0.0043 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Mn1—O6 | 2.1036 (15) | C3—C4 | 1.530 (3) |
| Mn1—O1 | 2.1444 (15) | C3—C3$^{iii}$ | 1.546 (3) |
| Mn1—O5$^{i}$ | 2.1695 (15) | C3—H3 | 0.9800 |
| Mn1—O1W | 2.2018 (16) | C4—O5 | 1.249 (2) |
| Mn1—O3 | 2.2230 (14) | C4—O6 | 1.257 (2) |
| Mn1—O4$^{i}$ | 2.2518 (14) | O3—H3A | 0.8199 |
| C1—O1 | 1.247 (2) | O4—Mn1$^{iv}$ | 2.2518 (14) |
| C1—O2 | 1.260 (2) | O4—H4 | 0.8198 |
| C1—C2 | 1.530 (2) | O5—Mn1$^{iv}$ | 2.1695 (15) |
| C2—O3 | 1.415 (2) | O1W—H1WA | 0.8215 |
| C2—C2$^{ii}$ | 1.542 (3) | O1W—H1WB | 0.8237 |
| C2—H2 | 0.9800 | O2W—H2WA | 0.8201 |
| C3—O4 | 1.429 (2) | O2W—H2WB | 0.8201 |
| O6—Mn1—O1 | 105.52 (6) | C2$^{ii}$—C2—H2 | 109.1 |
| O6—Mn1—O5$^{i}$ | 97.63 (6) | O4—C3—C4 | 109.91 (15) |
| O1—Mn1—O5$^{i}$ | 153.64 (6) | O4—C3—C3$^{iii}$ | 110.62 (18) |
| O6—Mn1—O1W | 92.32 (6) | C4—C3—C3$^{iii}$ | 113.12 (11) |
| O1—Mn1—O1W | 95.92 (6) | O4—C3—H3 | 107.7 |
| O5$^{i}$—Mn1—O1W | 95.55 (6) | C4—C3—H3 | 107.7 |
| O6—Mn1—O3 | 178.49 (5) | C3$^{iii}$—C3—H3 | 107.7 |
| O1—Mn1—O3 | 73.58 (5) | O5—C4—O6 | 125.50 (19) |
| O5$^{i}$—Mn1—O3 | 83.51 (5) | O5—C4—C3 | 119.39 (16) |
| O1W—Mn1—O3 | 86.58 (6) | O6—C4—C3 | 115.08 (17) |
| O6—Mn1—O4$^{i}$ | 96.86 (6) | C1—O1—Mn1 | 120.25 (12) |
| O1—Mn1—O4$^{i}$ | 90.96 (6) | C2—O3—Mn1 | 117.52 (10) |
| O5$^{i}$—Mn1—O4$^{i}$ | 73.67 (5) | C2—O3—H3A | 110.8 |
| O1W—Mn1—O4$^{i}$ | 166.64 (6) | Mn1—O3—H3A | 122.8 |
| O3—Mn1—O4$^{i}$ | 84.40 (5) | C3—O4—Mn1$^{iv}$ | 114.70 (10) |
| O1—C1—O2 | 124.68 (17) | C3—O4—H4 | 106.7 |
| O1—C1—C2 | 119.90 (16) | Mn1$^{iv}$—O4—H4 | 113.7 |
| O2—C1—C2 | 115.41 (16) | C4—O5—Mn1$^{iv}$ | 119.92 (12) |
| O3—C2—C1 | 108.55 (14) | C4—O6—Mn1 | 128.71 (13) |
| O3—C2—C2$^{ii}$ | 110.22 (11) | Mn1—O1W—H1WA | 125.2 |
| C1—C2—C2$^{ii}$ | 110.78 (18) | Mn1—O1W—H1WB | 103.9 |
| O3—C2—H2 | 109.1 | H1WA—O1W—H1WB | 96.1 |

| | | | |
|---|---|---|---|
| C1—C2—H2 | 109.1 | H2WA—O2W—H2WB | 108.4 |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4···O2W$^{v}$ | 0.82 | 1.81 | 2.628 (2) | 175 |
| O3—H3A···O2$^{vi}$ | 0.82 | 1.75 | 2.561 (2) | 173 |
| O1W—H1WA···O2$^{vii}$ | 0.82 | 2.04 | 2.643 (2) | 130 |
| O2W—H2WA···O5$^{iii}$ | 0.82 | 2.29 | 2.895 (2) | 131 |
| O2W—H2WB···O4$^{i}$ | 0.82 | 2.25 | 2.919 (3) | 140 |

Symmetry codes: (v) −*x*+1, *y*−1, −*z*+3/2; (vi) *x*, −*y*+1, *z*−1/2; (vii) *x*, *y*−1, *z*; (iii) −*x*+1, *y*, −*z*+3/2; (i) *x*, −*y*, *z*−1/2.

**Fig. 1**

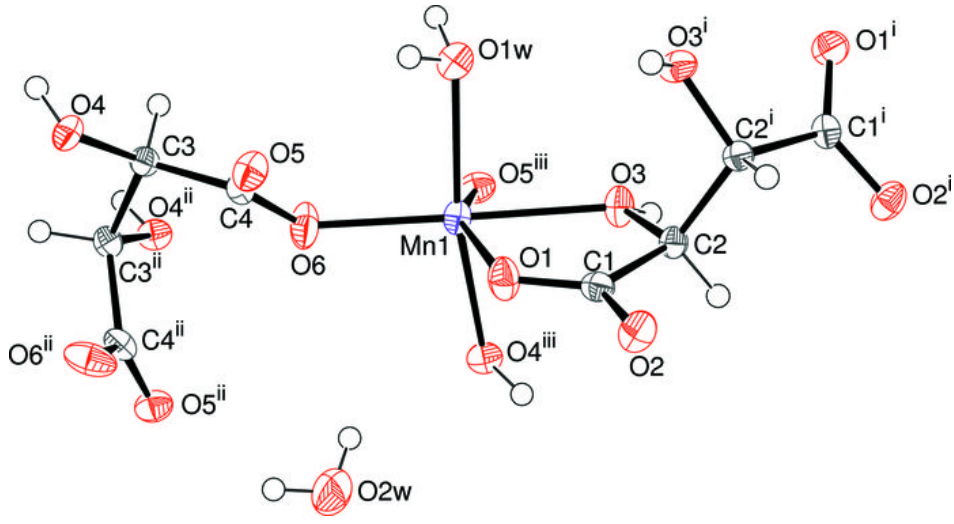
O1w
O3$^{i}$
O1$^{i}$
O4
C3
O5
C2$^{i}$
C1$^{i}$
O5$^{iii}$
O3
O2$^{i}$
O4$^{ii}$
C4
O6
Mn1
O1
C1
C2
C3$^{ii}$
O6$^{ii}$
C4$^{ii}$
O4$^{iii}$
O2
O5$^{ii}$
O2w

**Fig. 2**