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catena-Poly[[gallium(III)-bis[μ-D/L-tartrato(2−)]-gallium(III)-di-μ-hydroxido] dihydrate]

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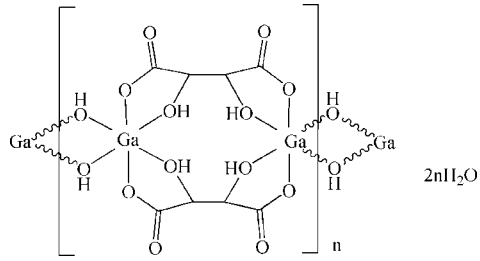
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.074; data-to-parameter ratio = 14.2.

In the title compound, $\{[Ga_2(C_4H_4O_6)_2(OH)_2]\cdot 2H_2O\}_n$, the Ga^{III} atom is located on a twofold rotation axis and is six-coordinated by two O atoms from bridging hydroxide groups and four O atoms from two symmetry-related tartrate units in a slightly distorted octahedral environment. Each tartrate unit binds to two Ga^{III} atoms as a bis-chelating bridging ligand by two pairs of hydroxide groups and an O atom of a carboxylate group. The Ga^{III} atoms are linked by two bridging hydroxide groups located on mirror planes. In this way a chain along the c axis is formed. Free water molecules on mirror planes are located between the chains and hold them together through hydrogen-bonding interactions, with O···O distances in the range 2.509 (3)–3.179 (5) Å.

Related literature

For the potential applications of coordination polymers in drug delivery, shape-selective sorption/separation and catalysis, see: Chen & Tong (2007); Zeng *et al.* (2009). For a description of their one-dimensional to three-dimensional architectures, see: Du & Bu (2009); Qiu & Zhu (2009). For our recent research on the synthesis of coordination polymers, see: Pan, Cheng & Bu (2010, 2011); Pan, Cheng & Hu (2010); Pan, Li *et al.* (2010); Pan, Ma *et al.* (2012); Wu *et al.* (2011).



Experimental

Crystal data

$[Ga_2(C_4H_4O_6)_2(OH)_2]\cdot 2H_2O$
M_r = 505.64
Orthorhombic, *Ibam*
a = 8.6830 (17) Å
b = 10.797 (2) Å
c = 16.158 (3) Å
V = 1514.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.65 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2002)
T_{min} = 0.421, T_{max} = 0.578
7524 measured reflections
897 independent reflections
756 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.074
S = 1.14
897 reflections
63 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ga1—O1	2.0102 (19)	Ga1—O4	1.9219 (18)
Ga1—O2	1.970 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H2···O3^{i}	0.89	1.64	2.509 (3)	163
O4—H4···O1W^{ii}	0.89	1.91	2.774 (5)	162
O1W—H1W···O2	0.89	2.56	3.179 (5)	127

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VN2042).

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supplementary materials

Acta Cryst. (2012). E**68**, m989–m990 [doi:10.1107/S1600536812028188]

catena-Poly[[gallium(III)-bis[μ-D/L-tartrato(2−)]-gallium(III)-di-μ-hydroxido] dihydrate]

Xiaojing Liu, Ruijing Tian, Cailing Zhang, Xia Zhi and Qinhe Pan

Comment

Recently, increasing attention has been paid to the design and synthesis of coordination polymers, because of their potential applications in drug delivery, shape-selective sorption/separation, and catalysis (Chen & Tong, 2007; Zeng *et al.*, 2009). Their structures vary from one-dimensional to three-dimensional architectures (Qiu & Zhu, 2009; Du & Bu, 2009). Our recent research interest has been focused on the synthesis of novel coordination polymers (Pan, Cheng & Bu, 2010, 2011; Pan, Cheng & Hu, 2010; Pan, Li *et al.*, 2010; Pan, Ma *et al.*, 2012; Wu *et al.* 2011). Here we present a Ga-containing coordination polymer with a one-dimensional chain structure.

As shown in Fig. 1, the asymmetric part of crystal structure of the title compound consists of half a Ga^{III} atom, half a tartrate anion, half a bridging hydroxide group, and half a free water molecule. The Ga^{III} atom is located on a twofold rotation axis and is six-coordinated by two O atoms from the bridging hydroxide groups, and four O atoms from two different tartrate units in a slightly distorted octahedral environment, with Ga—O bond distances in the range of 1.9219 (18) to 2.0102 (19) Å. The carboxylate groups of the tartrate are completely deprononated, the hydroxide group, however, is not. Chelated by the O1 atom from a hydroxide group and the O2 atom of neighboring carboxylate groups, each tartrate unit binds to two Ga^{III} atoms as a bis-chelating bridging ligand. Two Ga^{III} atoms and two tartrate units are linked to form a building unit, each building unit being surround by four O atoms of four different hydroxide groups, which is located on mirror, and linked two building units as the bridging hydroxide groups. In this way a one-dimensional chain along the *c* axis is formed by linking building units and the bridging hydroxide groups. Free water molecules reside between the chains while connecting them by hydrogen-bonding interactions as to form a three-dimensional supermolecular structure with O···O distances ranging from 2.509 (3)–3.179 (5) Å.

Experimental

In a typical synthesis, a mixture of Ga_2O_3 (0.047 g), D,*L*-tartaric acid (0.075 g), and H_2O (10 ml), was added to a 20 ml Teflon-lined reactor under autogenous pressure at 160 °C for 3 days, after which colorless prismatic shaped crystals were obtained.

Refinement

All H atoms were positioned geometrically (O—H = 0.89 Å, C—H = 0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s)

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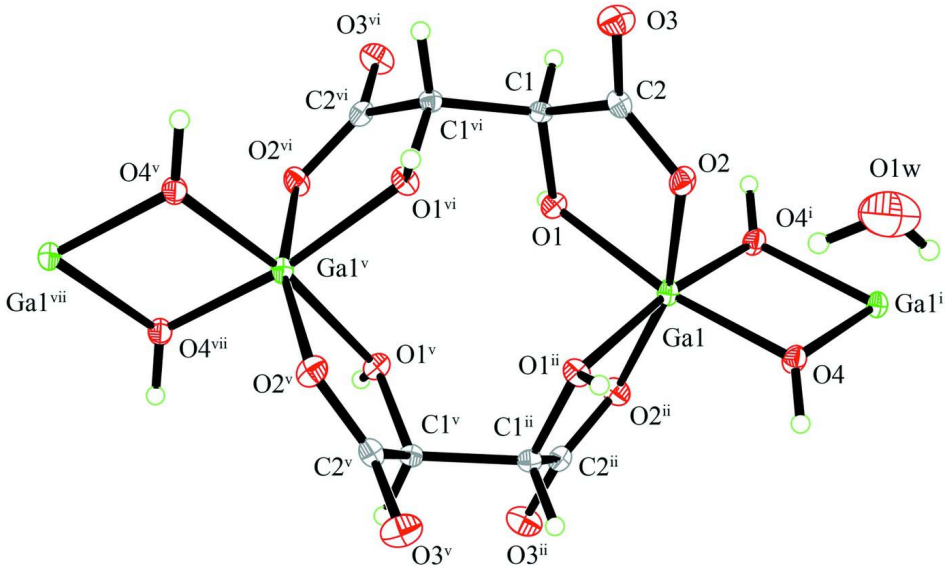

Figure 1

A view of the asymmetric unit of complex. Ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1 - *x*,1 - *y*,1 - *z*; (ii) 1 - *x*,1 - *y*,*z*; (v) *x*,1 - *y*,3/2 - *z*; (vi) 1 - *x*,*y*,3/2 - *z*; (vii) *x*,1 - *y*,1/2 + *z*.

catena-Poly[[gallium(III)-bis[*μ*-*D*/*L*-tartrato(2-)]- gallium(III)-di-*μ*-hydroxido] dihydrate]

Crystal data

$[Ga_2(C_4H_4O_6)_2(OH)_2]\cdot 2H_2O$
$M_r = 505.64$
Orthorhombic, *Ibam*
Hall symbol: -I22c
$a = 8.6830\ (17)$ Å
$b = 10.797\ (2)$ Å
$c = 16.158\ (3)$ Å
$V = 1514.8\ (5)$ Å^3
$Z = 4$
$F(000) = 1008$
$D_x = 2.217$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7524 reflections
$\theta = 3.0–27.4°$
$\mu = 3.65$ mm^{-1}
$T = 293$ K
Prism, colorless
0.3 × 0.2 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2002)
$T_{min} = 0.421$, $T_{max} = 0.578$
7524 measured reflections
897 independent reflections
756 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -11\rightarrow11$
$k = -13\rightarrow14$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
$S = 1.14$
897 reflections
63 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 2.6518P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ga1	0.5000	0.5000	0.59085 (2)	0.01685 (16)
O1	0.3677 (2)	0.42047 (17)	0.67803 (11)	0.0176 (4)
H2	0.3488	0.3398	0.6730	0.021*
O2	0.3489 (2)	0.63361 (18)	0.60822 (12)	0.0217 (4)
O3	0.1354 (2)	0.68818 (19)	0.67612 (14)	0.0290 (5)
O4	0.5962 (3)	0.5850 (3)	0.5000	0.0205 (6)
H4	0.6917	0.6148	0.5000	0.025*
C1	0.2355 (3)	0.4887 (2)	0.70276 (16)	0.0155 (5)
H1	0.1423	0.4434	0.6870	0.019*
C2	0.2388 (3)	0.6141 (3)	0.65840 (16)	0.0180 (6)
O1W	0.4116 (5)	0.8743 (5)	0.5000	0.0808 (15)
H1W	0.4511	0.8331	0.5428	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ga1	0.0208 (2)	0.0157 (2)	0.0140 (2)	−0.00133 (18)	0.000	0.000
O1	0.0212 (10)	0.0105 (9)	0.0212 (9)	0.0016 (8)	0.0037 (8)	0.0014 (8)
O2	0.0252 (11)	0.0174 (10)	0.0227 (10)	0.0019 (9)	0.0042 (9)	0.0071 (8)
O3	0.0280 (11)	0.0176 (10)	0.0414 (13)	0.0065 (9)	0.0058 (11)	0.0068 (9)
O4	0.0218 (15)	0.0234 (14)	0.0164 (13)	−0.0093 (12)	0.000	0.000
C1	0.0146 (12)	0.0139 (12)	0.0180 (13)	−0.0004 (11)	−0.0003 (11)	0.0009 (11)
C2	0.0211 (14)	0.0148 (13)	0.0180 (13)	0.0005 (11)	−0.0037 (12)	−0.0003 (10)
O1W	0.048 (3)	0.105 (4)	0.089 (4)	0.008 (3)	0.000	0.000

Geometric parameters (Å, º)

Ga1—O1	2.0102 (19)	O2—C2	1.271 (3)
Ga1—O2	1.970 (2)	O3—C2	1.236 (3)
Ga1—O4^{i}	1.9219 (18)	O4—Ga1^{i}	1.9219 (17)
Ga1—O4	1.9219 (18)	O4—H4	0.8900
Ga1—O2^{ii}	1.970 (2)	C1—C2	1.532 (4)
Ga1—O1^{ii}	2.0102 (19)	C1—C1^{iii}	1.546 (5)
Ga1—Ga1^{i}	2.9358 (10)	C1—H1	0.9800
O1—C1	1.421 (3)	O1W—H1W	0.8900
O1—H2	0.8900		
O4^{i}—Ga1—O4	80.41 (12)	O1^{ii}—Ga1—Ga1^{i}	134.49 (6)
O4^{i}—Ga1—O2^{ii}	92.78 (10)	O1—Ga1—Ga1^{i}	134.49 (6)
O4—Ga1—O2^{ii}	99.74 (10)	C1—O1—Ga1	115.90 (15)
O4^{i}—Ga1—O2	99.74 (10)	C1—O1—H2	112.6
O4—Ga1—O2	92.78 (10)	Ga1—O1—H2	117.4
O2^{ii}—Ga1—O2	163.61 (11)	C2—O2—Ga1	118.06 (17)
O4^{i}—Ga1—O1^{ii}	170.89 (9)	Ga1^{i}—O4—Ga1	99.59 (12)
O4—Ga1—O1^{ii}	94.76 (8)	Ga1^{i}—O4—H4	125.3
O2^{ii}—Ga1—O1^{ii}	80.36 (7)	Ga1—O4—H4	125.3
O2—Ga1—O1^{ii}	88.15 (8)	O1—C1—C2	108.2 (2)
O4^{i}—Ga1—O1	94.76 (8)	O1—C1—C1^{iii}	111.05 (17)
O4—Ga1—O1	170.89 (9)	C2—C1—C1^{iii}	108.8 (3)
O2^{ii}—Ga1—O1	88.15 (8)	O1—C1—H1	109.6
O2—Ga1—O1	80.36 (7)	C2—C1—H1	109.6
O1^{ii}—Ga1—O1	91.02 (11)	C1^{iii}—C1—H1	109.6
O4^{i}—Ga1—Ga1^{i}	40.20 (6)	O3—C2—O2	125.9 (3)
O4—Ga1—Ga1^{i}	40.20 (6)	O3—C2—C1	116.7 (2)
O2^{ii}—Ga1—Ga1^{i}	98.19 (6)	O2—C2—C1	117.3 (2)
O2—Ga1—Ga1^{i}	98.19 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H2···O3^{iv}	0.89	1.64	2.509 (3)	163
O4—H4···O1*W*^{v}	0.89	1.91	2.774 (5)	162
O1*W*—H1*W*···O2	0.89	2.56	3.179 (5)	127

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