

Hexaaquagallium(III) trinitrate trihydrate

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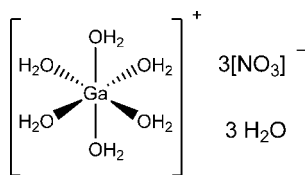
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{O}-\text{N}) = 0.002$ Å; R factor = 0.021; wR factor = 0.058; data-to-parameter ratio = 11.1.

The title compound, $[\text{Ga}(\text{H}_2\text{O})_6](\text{NO}_3)_3 \cdot 3\text{H}_2\text{O}$, is isostructural to other known M^{III} nitrate hydrates ($M = \text{Al}, \text{Cr}, \text{Fe}$). The structure contains two distinct octahedral $\text{Ga}(\text{OH}_2)_6$ units (each of $\bar{1}$ symmetry) which are involved in intermolecular hydrogen bonding with the three nitrate anions and three water molecules within the asymmetric unit.

Related literature

For the aluminium analogue, see: Lazar, Ribár, Divjaković & Mészáros (1991). For the chromium analogue, see: Lazar, Ribár & Prelesnik (1991). For the iron analogue, see: Hair & Beattie (1977). For ionic radii, see: Shannon & Prewitt (1969). Gallium nitrate, used in the preparation, easily forms super-saturated solutions, see: Rudolph *et al.* (2002), and hence the sample was cooled to 248 K and a seed crystal was introduced to initiate crystallization.



Experimental

Crystal data

$[\text{Ga}(\text{H}_2\text{O})_6](\text{NO}_3)_3 \cdot 3\text{H}_2\text{O}$
 $M_r = 417.89$
 Monoclinic, $P2_1/c$
 $a = 13.9609$ (6) Å
 $b = 9.6498$ (5) Å
 $c = 10.9743$ (5) Å
 $\beta = 95.448$ (1)°

$V = 1471.78$ (12) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.97$ mm⁻¹
 $T = 296$ K
 $0.40 \times 0.34 \times 0.29$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\text{min}} = 0.479$, $T_{\text{max}} = 0.564$

10587 measured reflections
 3037 independent reflections
 2509 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.058$
 $S = 1.05$
 3037 reflections
 274 parameters
 18 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O18—H18···O8	0.801 (16)	2.26 (2)	2.9348 (18)	142 (2)
O16—H14···O18	0.825 (15)	2.072 (15)	2.8732 (19)	163.8 (19)
O5—H10···O7	0.823 (16)	1.908 (17)	2.7052 (17)	163 (2)
O1—H1···O16	0.814 (15)	1.846 (16)	2.6474 (16)	168 (2)
O4—H7···O14	0.809 (15)	1.833 (15)	2.6399 (15)	175 (2)
O5—H9···O17	0.810 (16)	1.869 (16)	2.676 (2)	174 (2)
O18—H17···O14	0.816 (16)	2.082 (17)	2.8729 (18)	163 (2)
O3—H6···O15 ⁱ	0.814 (15)	1.903 (16)	2.7150 (16)	175 (2)
O1—H2···O10 ^j	0.808 (15)	1.848 (16)	2.6545 (16)	175 (2)
O2—H4···O16 ^k	0.790 (16)	1.901 (16)	2.6895 (18)	175 (2)
O4—H8···O17 ⁱⁱ	0.821 (15)	1.816 (15)	2.6312 (16)	171 (2)
O17—H15···O9 ⁱⁱⁱ	0.808 (15)	1.977 (16)	2.7791 (19)	171 (2)
O3—H5···O13 ⁱⁱⁱⁱ	0.792 (15)	1.961 (16)	2.7454 (16)	171 (2)
O6—H12···O12 ^{iv}	0.796 (15)	1.926 (16)	2.7179 (16)	174 (2)
O16—H13···O18 ^v	0.820 (16)	1.934 (16)	2.7525 (19)	177 (3)
O6—H11···O11 ^{vi}	0.800 (15)	1.895 (16)	2.6938 (17)	176 (2)
O2—H3···O8 ^{vii}	0.794 (15)	1.943 (16)	2.7269 (17)	169 (2)
O17—H16···O7 ^{viii}	0.802 (16)	2.026 (18)	2.7675 (18)	154 (2)

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2076).

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