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Key indicators

Single-crystal X-ray study
 $T = 291$ K
Mean $\sigma(r-O) = 0.005$ Å
Disorder in main residue
 R factor = 0.029
 wR factor = 0.089
Data-to-parameter ratio = 9.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Nonaquayttrium(III) tris(bromate)

In the structure of the title compound, $[\text{Y}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$, the yttrium(III) ion is surrounded by six equidistant water molecules forming a trigonal prism, which is capped by three more distant water molecules. The Y^{III} ion lies on a special position ($2c$) with crystallographically imposed $\bar{6}m2$ symmetry. The title compound is isotypic with other $[\text{Ln}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$ ($\text{Ln} = \text{Pr}, \text{Sm}, \text{Tb}$ and Yb) compounds, and the bromate anions are disordered in these structures. Relatively strong hydrogen bonds between the bromate anions and the water molecules stabilize the trigonal prism.

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Comment

The title compound, $[\text{Y}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$, (I), has been studied with the aim of investigating the nature of the coordination geometries of water molecules around yttrium(III) ions and to make a comparison with the related structures of the analogous nonahydrated yttrium(III) trifluoromethanesulfonate and ethylsulfate compounds, including hydrogen bonding and anion effects. The nonahydrated lanthanoid(III) complexes with the anions bromate (Helmholz, 1939; Sikka, 1969; Albertsson & Elding, 1977; Moret *et al.*, 1991), ethylsulfate (Broach *et al.*, 1979; Gerkin & Reppart, 1984) and trifluoromethanesulfonate (Harrowfield *et al.*, 1983; Chatterjee *et al.*,

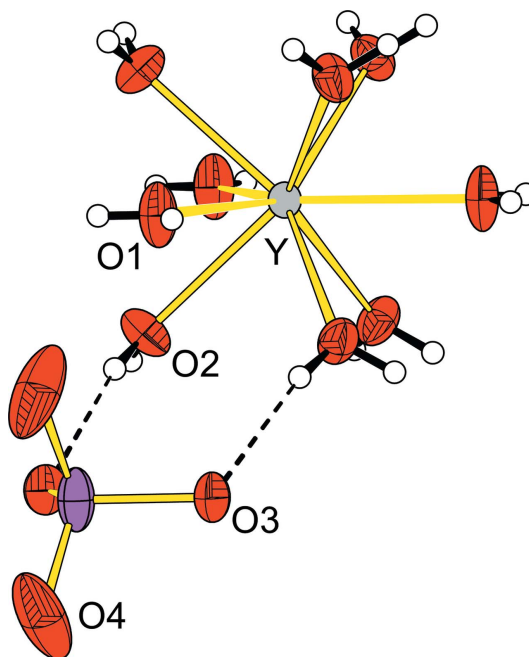


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids. H atoms are shown as circles of arbitrary radii. Hydrogen bonds are indicated by dashed lines.

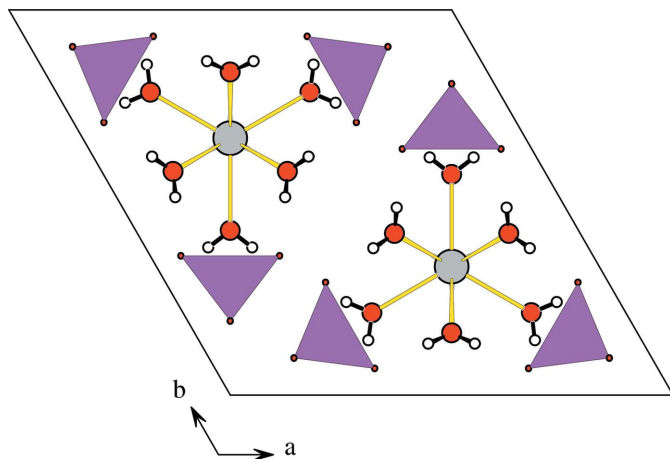


Figure 2
A packing diagram for (I), in a view along the *c* axis, with bromate anions shown as polyhedra.

1988; Abbasi *et al.*, 2005) represent a homeotypic series with tricapped trigonal-prismatic coordination polyhedra around Ln^{3+} . Their structures have previously been discussed in detail. The isotopic $[\text{Ln}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$ ($\text{Ln} = \text{Pr}, \text{Sm}, \text{Tb}$ and Yb) compounds belong to the same space group as the title compound, *viz.* $P6_3/mmc$, while for the isoformular compound $[\text{Ho}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$, the space group is reported to be $Cmcm$ (Gerkin & Reppart, 1987). However, the diffraction intensity data for this last compound, collected at ambient and low temperatures, were not sufficient to determine the space group unambiguously (Gerkin & Reppart, 1987).

In (I), the bromate anions are disordered, so that each Br atom is surrounded by two fully occupied (O3) and two half-occupied (O4) O-atom sites in a nearly tetrahedral configuration (Fig. 1). Atom O4 has a relatively large displacement parameter and is located in two split positions in close contact with the corresponding O atoms from other bromate anions [$\text{O4} \cdots \text{O4}(-x, -x + y, 2 - z) = 2.044(2) \text{ \AA}$].

The hydrogen-bonding distances between the slightly less polarized capping water molecules and the bromate O atoms are found to be slightly longer than those between the prismatic water molecules and the anions (Table 2). All H atoms of the capping water molecules are located in the plane of the capping O atoms (see packing view, Fig. 2), whereas in nonahydrated yttrium(III) trifluoromethanesulfonate and ethylsulfate, they are perpendicular to the capping plane, so that the hydrogen bonds are different (Harrowfield *et al.*, 1983).

Experimental

Compound (I) was synthesized by dissolving KBrO_3 (Aldrich, 99.8%) in a solution of $\text{Y}(\text{ClO}_4)_3$ (Aldrich 99.9%, 40 wt% in water). The precipitated KClO_4 was filtered off and crystals of (I) suitable for data collection were obtained after repeated recrystallization from water.

Crystal data

$[\text{Y}(\text{H}_2\text{O})_9](\text{BrO}_3)_3$
 $M_r = 634.78$
Hexagonal, $P6_3/mmc$
 $a = 11.7237(16) \text{ \AA}$
 $c = 6.6855(9) \text{ \AA}$
 $V = 795.78(19) \text{ \AA}^3$
 $Z = 2$

$D_x = 2.649 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 11.28 \text{ mm}^{-1}$
 $T = 291(2) \text{ K}$
Needle, colourless
 $0.40 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Stoe IPDS area-detector diffractometer
 φ scans
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997)
 $T_{\min} = 0.01, T_{\max} = 0.40$

12059 measured reflections
336 independent reflections
311 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.085$
 $\theta_{\max} = 26.2^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.089$
 $S = 1.23$
336 reflections
34 parameters
Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 3.0946P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.70 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.62 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (\AA).

Y—O1	2.434 (7)	Br—O4	1.533 (15)
Y—O2	2.371 (4)	Br—O3	1.655 (4)

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1 \cdots O3 ⁱ	0.73 (9)	2.15 (9)	2.869 (8)	168
O2—H2 \cdots O3 ⁱⁱ	0.78 (5)	2.06 (5)	2.837 (6)	169

Symmetry codes: (i) $x - y, x, -z + 1$; (ii) $-y + 1, x - y + 1, z - 1$.

H atoms were located in difference density maps and their coordinates were refined freely, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 1997); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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References

- Abbasi, A., Lindqvist-Reis, P., Eriksson, L., Sandström, D., Lidin, S., Persson, I. & Sandström, M. (2005). *Chem. Eur. J.* **11**, 4065–4077.
Albertsson, J. & Elding, I. (1977). *Acta Cryst.* **B33**, 1460–1469.
Brandenburg, K. (1999). *DIAMOND* (Version 2.1e). Crystal Impact GbR, Bonn, Germany.

- Broach, R. W., Williams, J. M., Felcher, G. P. & Hinks, D. G. (1979). *Acta Cryst.* **B35**, 2317–2321.
- Chatterjee, A., Maslen, E. N. & Watson, K. J. (1988). *Acta Cryst.* **B44**, 381–386.
- Gerkin, R. E. & Reppart, W. J. (1984). *Acta Cryst.* **C40**, 781–786.
- Gerkin, R. E. & Reppart, W. J. (1987). *Acta Cryst.* **C43**, 623–631.
- Harrowfield, J. M., Kepert, D. L. & Patrick, J. M. (1983). *Aust. J. Chem.* **36**, 483–492.
- Helmholz, J. (1939). *J. Am. Chem. Soc.* **61**, 1544–1550.
- Moret, E., Nicolo, F. & Bünzli, J.-C. G. (1991). *J. Less Common Met.* **171**, 273–300.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sikka, S. K. (1969). *Acta Cryst.* **A25**, 621–626.
- Stoe & Cie (1997). *IPDS Software* (Version 2.87) and *X-RED* (Version 1.09). Stoe & Cie GmbH, Darmstadt, Germany.