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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(c-O) = 0.002$  Å  
 $R$  factor = 0.030  
 $wR$  factor = 0.073  
Data-to-parameter ratio = 32.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Pentaaquahydroxoscandium(III) dibromide,  
[Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]Br<sub>2</sub>

[Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]Br<sub>2</sub> is a scandium(III) halide compound that contains centrosymmetric [Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]<sub>2</sub><sup>4+</sup> dimeric cationic units built from two edge-sharing (hydroxo-bridged) symmetrically equivalent Sc(H<sub>2</sub>O)<sub>5</sub>(OH)<sub>2</sub> polyhedra. The mean Sc—O bond length is 2.156 Å. The hydrogen bonds (O···Br) are of low strength. All atoms are in general positions.

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## Comment

As part of work on the crystallochemical behaviour of Sc<sup>III</sup> in inorganic compounds, pentaaquahydroxoscandium(III) dibromide, [Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]Br<sub>2</sub>, (I), was obtained. Although a compound with this formula has been reported in the literature (Petru & Kutek, 1960; Arkhangel'skii *et al.*, 1972), neither the crystal symmetry nor the crystal structure were given.

The crystal structure of (I) contains centrosymmetric dimeric cationic [Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]<sub>2</sub><sup>4+</sup> units, counterbalanced by Br<sup>−</sup> anions. The cationic unit is built from two edge-sharing symmetrically equivalent Sc(H<sub>2</sub>O)<sub>5</sub>(OH)<sub>2</sub> polyhedra (Fig. 1). The polyhedron may be described as a monocapped (by O1) trigonal antiprism. The two OH groups (O1—H1) act as hydroxo-bridges between the two Sc-centred polyhedra (Fig. 2).

Practically identical dimeric cationic units also occur in orthorhombic [Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]<sub>2</sub>X<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>, where X = Br or Cl (Ilyukhin & Petrosyants, 1994; Ripert *et al.*, 1999; see also Petrosyants & Ilyukhin, 2004). In contrast, the crystal structures of monoclinic [Sc(H<sub>2</sub>O)<sub>7</sub>]X<sub>3</sub>, where X = Br or Cl (Lim *et al.*, 2000), contain isolated Sc(H<sub>2</sub>O)<sub>7</sub> polyhedra.

The mean Sc—O bond length in (I) is 2.156 Å (Table 1), in accordance with the grand mean Sc—O bond length of 2.17 (7) Å given for heptacoordinated Sc in a review of Sc

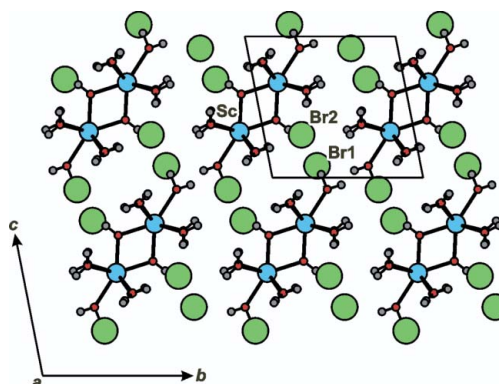
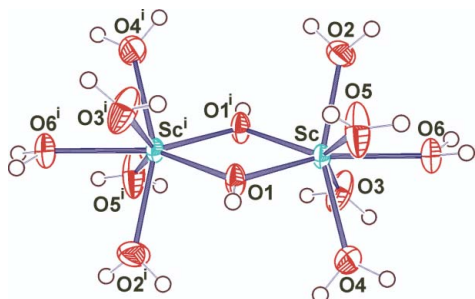


Figure 1

A view of the crystal structure of (I) along [100]. Dimeric [Sc(H<sub>2</sub>O)<sub>5</sub>(OH)]<sub>2</sub><sup>4+</sup> cationic units are bonded to Br<sup>−</sup> anions *via* weak hydrogen bonds. Sc atoms are shown in turquoise, Br atoms in green, O atoms in red and H atoms in grey. The unit cell is outlined. All atoms are shown as spheres of arbitrary radii.

**Figure 2**

A view of the dimeric  $[\text{Sc}(\text{H}_2\text{O})_5(\text{OH})]_2^{4+}$  cationic unit in (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. [Symmetry code: (i)  $-x, -y, -z$ .]

compounds by Serezhkin *et al.* (2003). The Sc—OH bonds are distinctly shorter than the Sc—H<sub>2</sub>O bonds, equivalent to the situation in  $[\text{Sc}(\text{H}_2\text{O})_5(\text{OH})]_2\text{X}_4(\text{H}_2\text{O})_2$ , where  $\text{X} = \text{Br}$  or  $\text{Cl}$  (Ilyukhin & Petrosyants, 1994; Ripert *et al.*, 1999), and also in agreement with the observations of Serezhkin *et al.* (2003).

The hydrogen bonds are of low strength, as shown by  $\text{O} \cdots \text{Br}$  distances between about 3.24 and 3.41 Å (Table 2).

## Experimental

Compound (I) was prepared by mixing  $\text{Sc}_2\text{O}_3$ , 48%<sub>wt</sub> HBr, concentrated  $\text{HNO}_3$  and distilled water at room temperature (the volume ratios are unknown, but the two acids were added in excess quantities). On slow evaporation of the acidic aqueous solution, compound (I) formed as colourless rounded tabular crystals, stable under ambient conditions. The crystals were accompanied by minor amounts of thin crusts of  $[\text{Sc}(\text{H}_2\text{O})_5(\text{OH})]_2\text{Br}_4(\text{H}_2\text{O})_2$  (Ilyukhin & Petrosyants, 1994; Ripert *et al.*, 1999).

### Crystal data

$[\text{Sc}(\text{H}_2\text{O})_5(\text{OH})]\text{Br}_2$	$V = 468.3 (2) \text{ \AA}^3$
$M_r = 311.87$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 2.212 \text{ Mg m}^{-3}$
$a = 7.412 (1) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.368 (2) \text{ \AA}$	$\mu = 9.29 \text{ mm}^{-1}$
$c = 8.627 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 95.12 (3)^\circ$	Fragment, colourless
$\beta = 114.56 (3)^\circ$	$0.17 \times 0.15 \times 0.10 \text{ mm}$
$\gamma = 101.33 (3)^\circ$	

### Data collection

Nonius KappaCCD area-detector diffractometer	$T_{\min} = 0.301, T_{\max} = 0.457$ (expected range = 0.260–0.395)
$\varphi$ and $\omega$ scans	8112 measured reflections
Absorption correction: multi-scan (SCALEPACK; Otwinowski <i>et al.</i> , 2003)	4082 independent reflections 3219 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.021$ $\theta_{\text{max}} = 34.9^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.15P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.073$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.98 \text{ e \AA}^{-3}$
4082 reflections	$\Delta\rho_{\text{min}} = -0.87 \text{ e \AA}^{-3}$
127 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 1997)
All H-atom parameters refined	Extinction coefficient: 0.0166 (13)

**Table 1**

Selected bond lengths (Å).

Sc—O1	2.0485 (15)	Sc—O5	2.2024 (19)
Sc—O1 <sup>i</sup>	2.0824 (15)	Sc—O4	2.2032 (19)
Sc—O2	2.1591 (19)	Sc—O6	2.2228 (18)
Sc—O3	2.1724 (19)		

Symmetry code: (i)  $-x + 2, -y, -z + 1$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

$D\text{—H}\cdots A$	$D\text{—H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
O1—H1 $\cdots$ Br1 <sup>i</sup>	0.85 (2)	2.52 (2)	3.3532 (17)	165 (3)
O2—H2 $\cdots$ Br1 <sup>ii</sup>	0.87 (2)	2.39 (2)	3.236 (2)	165 (3)
O2—H3 $\cdots$ Br2 <sup>iii</sup>	0.88 (2)	2.54 (2)	3.392 (2)	162 (3)
O3—H4 $\cdots$ Br1 <sup>iv</sup>	0.89 (2)	2.38 (2)	3.265 (2)	173 (3)
O3—H5 $\cdots$ Br2	0.89 (2)	2.54 (2)	3.407 (2)	165 (3)
O4—H6 $\cdots$ Br2 <sup>v</sup>	0.88 (2)	2.53 (2)	3.371 (2)	161 (3)
O4—H7 $\cdots$ Br2 <sup>vi</sup>	0.88 (2)	2.40 (2)	3.280 (2)	174 (4)
O5—H8 $\cdots$ Br2 <sup>i</sup>	0.88 (2)	2.44 (2)	3.312 (2)	170 (4)
O5—H9 $\cdots$ Br1 <sup>v</sup>	0.86 (2)	2.48 (2)	3.302 (2)	160 (4)
O6—H10 $\cdots$ Br2 <sup>iv</sup>	0.89 (2)	2.41 (2)	3.2940 (18)	175 (3)
O6—H11 $\cdots$ Br1 <sup>v</sup>	0.87 (2)	2.42 (3)	3.2413 (18)	156 (4)

Symmetry codes: (i)  $-x + 2, -y, -z + 1$ ; (ii)  $-x + 2, -y, -z$ ; (iii)  $x + 1, y, z$ ; (iv)  $-x + 1, -y, -z$ ; (v)  $x, y - 1, z$ ; (vi)  $-x + 1, -y, -z + 1$ .

All O—H distances were restrained to a length of 0.90 (2) Å, and the  $U_{\text{iso}}(\text{H})$  values were freely refined.

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski *et al.*, 2003); data reduction: *SCALEPACK* and *DENZO* (Otwinowski *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1999) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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