(1994). A white powder sample of $LiBeAsO_4.H_2O$ was carefully packed into a 2 × 1 cm flat-plate sample holder and mounted horizontally in air. Unfiltered Cu $K\alpha$ radiation (λ = 1.54178 Å) was used to collect the step-scan diffraction data. No monochromation was used.

Starting unit-cell parameters were obtained by unit-cell powder refinements and starting atomic coordinates were obtained from the structure determination of $LiZnPO_4.H_2O$ (Harrison, Gier, Nicol & Stucky, 1995) with Be substituting for Zn and As replacing P. Proton positions were not included in the structural model, and Be—O bond-distance restraints [Be—O = 1.63 (2) Å] were used to stabilize the refinement. The relative weight of these extra observations was progressively reduced as the model converged. The Rietveld refinement progressed smoothly, with the usual profile parameters (scale factor, zero-point error, pseudo-Voigt peak-width variation parameters, six-term Fourier-cosine series background coefficients, unit-cell parameters) treated as least-squares variables in the usual fashion. Refined peak-shape descriptors of GU = 0, GV = 0, GW = 19.2 (7), LX = 2.0 (3) and LY = 16.4 (9) resulted. Refined background coefficients were 3.2 (5), 0.8 (5), −4 (2), 7 (3), −5 (2) and 2.1 (5). All atom positions and isotropic displacement factors [$U_{\rm iso}$(Li) fixed at 0.01 Å^2] were refined subject to the constraints $U_{\rm iso}$(Be) = $U_{\rm iso}$(As) and an atom-type $U_{\rm iso}$ for the framework O atoms. No corrections for preferred orientation, extinction or absorption were applied.

Program(s) used to refine structure: *GSAS* (Larson & Von Dreele, 1990). Molecular graphics: *ORTEP*II (Johnson, 1976) and *STRUPLO* (Fischer, 1985).

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Lists of raw power data and complete geometry have been deposited with the IUCr (Reference: BR1093). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Strontium Dibromide Hexahydrate

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Abstract

The structure of $SrBr_2.6H_2O$ has been solved by single-crystal X-ray analysis. Each Sr atom has tricapped trigonal prismatic coordination geometry involving six bridging and three terminal water molecules. The bridging arrangement results in a linear polymeric cation $[Sr(H_2O)_6]_n^{2n+}$ with charges balanced by Br^- ions in the lattice.

Comment

The title compound is readily crystallized from hot solutions of Sr^{2+} in HBr and is often formed as an impurity in the preparation of binary metal bromides. Several crystallographic studies of anhydrous (Sass, Brackett & Brackett, 1963; Smeggil & Eick, 1971) and monohydrated (Dyke & Sass, 1964; Engelen, Freiburg & Lutz, 1983; Lutz, Buchmeier & Engelen, 1987) strontium bromides have been carried out. Early studies (Herrmann, 1931; Jensen, 1940) showed that the title compound was likely to be isostructural with the analogous chloride. The present study, however, constitutes the first full determination of the structure of $SrBr_2.6H_2O$.

The title compound contains nine-coordinate Sr in tricapped trigonal prismatic coordination geometry (Fig. 1) involving six bridging and three terminal water molecules. The bridging water molecules at the apices of the trigonal prism link the Sr^{2+} ions at the centre of each prism, resulting in a linear cationic polymer, $[Sr(H_2O)_6]_n^{2n+}$, which is balanced in charge by Br^- ions in the lattice. The Br^- ions are hydrogen bonded to the water molecules.

$SrBr_2.6H_2O$ is isostructural with $CaBr_2.6H_2O$ (Leclaire & Borel, 1977). The strontium and calcium dichloride hexahydrates are also isostructural. The bridging and terminal contacts to water in these compounds are compared in Table 3.

It is clear that the interatomic distances observed in $SrBr_2.6H_2O$ compare well with those found in $SrCl_2.6H_2O$, particularly in the case of the bridging contacts. The structure of $MgBr_2.6H_2O$ (Andress & Gundermann, 1934) is also known, but contains isolated $[Mg(H_2O)_6]^{2+}$ ions with no bridging water molecules. The hydrogen-bonding contacts in the title compound lie in the range 3.35–3.37 Å, and are comparable to those observed in $HBr.3H_2O$ (Lundgren, 1970).

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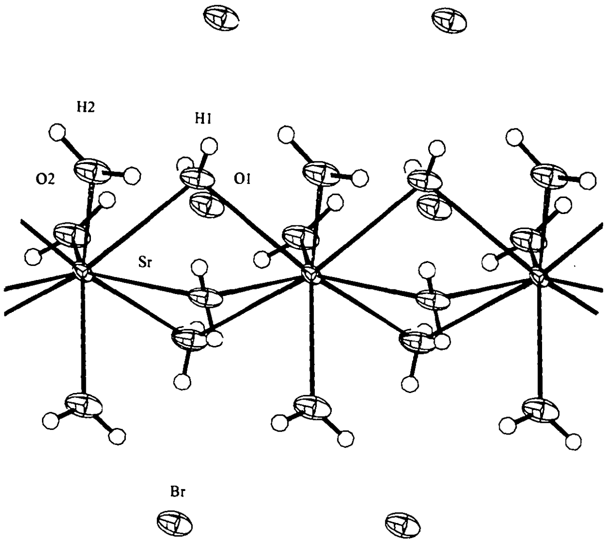

Fig. 1. The structure of $SrBr_2.6H_2O$. Displacement ellipsoids are shown at the 50% probability level.

Experimental

$SrBr_2.6H_2O$ was prepared by dissolving $SrCO_3$ in concentrated HBr and boiling to minimal volume. White needles formed on cooling which were dried over silica gel *in vacuo*.

Crystal data

$SrBr_2.6H_2O$
$M_r = 355.54$
Trigonal
$P321$
$a = 8.204\,(3)$ Å
$c = 4.1590\,(10)$ Å
$V = 242.42\,(14)$ Å^3
$Z = 1$
$D_x = 2.435$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 10$–$14°$
$\mu = 13.779$ mm^{-1}
$T = 291\,(2)$ K
Prism
$0.40 \times 0.13 \times 0.13$ mm
White

Data collection

Enraf–Nonius CAD-4 four-circle diffractometer
$2\theta/\omega$ scans
Absorption correction: *DIFABS* (Walker & Stuart, 1983)
$T_{min} = 0.739$, $T_{max} = 0.899$
282 measured reflections
240 independent reflections

194 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.0228$
$\theta_{max} = 27.92°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 5$
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0294$
$wR(F^2) = 0.0750$
$S = 0.796$

$(\Delta/\sigma)_{max} = 0.530$
$\Delta\rho_{max} = 0.478$ e Å^{-3}
$\Delta\rho_{min} = -1.318$ e Å^{-3}
Extinction correction: none

240 reflections
24 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0782P)^2 + 0.5214P]$
where $P = (F_o^2 + 2F_c^2)/3$

Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Sr	0	0	0	0.0191 (3)
Br	1/3	2/3	−0.4405 (2)	0.0330 (4)
O1	0.7874 (8)	0	1/2	0.0282 (14)
O2	0.3112 (9)	0	0	0.034 (2)

Table 2. *Selected geometric parameters* (Å, °)

Sr—O2^i	2.553 (8)	Br···O1^{iii}	3.351 (5)
Sr—O1^{ii}	2.714 (4)	Br···O2^{iii}	3.371 (4)
O2^i—Sr—O2	120.0	O1^{ii}—Sr—O1^{iv}	142.52 (9)
O2^i—Sr—O1^{ii}	129.98 (11)	O1^{iv}—Sr—O1^{v}	67.6 (2)
O2—Sr—O1^{ii}	71.26 (4)	O1^{iv}—Sr—O1^{vi}	100.0 (2)

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

Table 3. *Comparison of bond distances* (Å) *in* $MX_2.6H_2O$ (M = Ca, Sr; X = Cl, Br)

	M—OH_2 bridging	M—OH_2 terminal
$SrBr_2.6H_2O^a$	2.714 (4)	2.553 (8)
$SrCl_2.6H_2O^b$	2.715 (1)	2.570 (2)
$SrCl_2.6H_2O^c$	2.709 (2)	2.562 (4)
$CaBr_2.6H_2O^d$	2.622 (7)	2.466 (9)
$CaCl_2.6H_2O^b$	2.594 (1)	2.453 (1)
$CaCl_2.6H_2O^d$	2.590 (2)	2.451 (3)

References: (*a*) this work; (*b*) Agron & Busing (1986); (*c*) English & Nassimbeni (1984); (*d*) Leclaire & Borel (1977).

Data collection and cell refinement: *CAD*-4/*PC* (Enraf–Nonius, 1992). Data reduction: *CAD*-4 (Davies, 1976). The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1990) and refined using *SHELXL*93 (Sheldrick, 1993). H atoms were located using difference Fourier techniques. The absolute configuration was determined by calculation of the Flack parameter [$x = -0.04\,(6)$; Flack, 1983]. Molecular graphics: *SNOOPI* (Davies, 1983).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BR1090). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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